Results of Proficiency Test
Acetone
September 2021

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 Acetone in accordance with the latest version of ASTM D329 once every two years. During the annual proficiency testing program 2021/2022 it was decided to continue the proficiency tests for the analysis of Acetone.

In this interlaboratory study 26 laboratories in 14 different countries registered for participation. See appendix 2 for the number of participants per country. In this report the results of the Acetone 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 a one bottle of 1 liter filled with Acetone labelled #21165.
The participants were requested to report rounded and unrounded test results. The unrounded test results were preferably used for statistical evaluation.

2.1 QUALITY SYSTEM

The Institute for Interlaboratory Studies in Spijkenisse, the Netherlands, has implemented a quality system based on ISO/IEC17043:2010. 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 50 liters Acetone was obtained from a local supplier. After homogenization 50 amber glass bottles of 1L were filled and labelled #21165.
The homogeneity of the subsamples was checked by determination by determination of Density at 20°C in accordance D4052 and Water in accordance with ASTM E203 on 4 stratified randomly selected subsamples.

	Density at 20°C in kg/L	Water in %M/M
sample #21165-1	0.79043	0.1920
sample #21165-2	0.79045	0.1920
sample #21165-3	0.79043	0.1910
sample #21165-4	0.79046	0.1910

Table 1: homogeneity test results of subsamples #21165

From the above test results the repeatabilities were calculated and compared with 0.3 times the corresponding reproducibility of the reference test methods in agreement with the procedure of ISO13528, Annex B2 in the next table.

	Density at 20°C in kg/L	Water in %M/M
r (observed)	0.00004	0.0016
reference test method	ISO12185:96	ASTM E203:16
0.3 x R (reference test method)	0.00015	0.023

Table 2: evaluation of repeatabilities of subsamples #21165

The calculated repeatabilities are in agreement with 0.3 times the corresponding reproducibility of the reference test methods. Therefore, homogeneity of the subsamples was assumed.

To each of the participating laboratories one sample Acetone labelled #21165 was sent on August 25, 2021. An SDS was added to the sample package.

2.5 STABILITY OF THE SAMPLES

The stability of Acetone 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: Acidity as Acetic acid, Aldehydes, Appearance, Inorganic Chloride as Cl, Color Pt/Co, Density at 20°C, Specific Gravity 20/20°C, Distillation (IBP, 50% recovered, DP and Distillation Range), Miscibility with water (Hydrocarbons), Nonvolatile matter, Permanganate Time Test at 25°C, Purity by GC on dry basis, Diacetone alcohol, Mesityloxide, Methanol, Refractive Index at 20°C and Water.

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

To get comparable test results a detailed report form and a letter of instructions are prepared. On the report form the reporting units are given as well as the appropriate 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 original test results are placed under 'Remarks' in the test result tables in appendix 1. Test results that came in after the deadline were not taken into account in this screening for suspect data and thus these participants were not requested for checks.

3.1 STATISTICS

The protocol followed in the organization of this proficiency test was the one as described for proficiency testing in the report ‘iis Interlaboratory Studies: Protocol for the Organisation, Statistics and Evaluation’ of June 2018 (iis-protocol, version 3.5).
For the statistical evaluation the *unrounded* (when available) figures were used instead of the rounded test results. Test results reported as ‘<…’ or ‘>…’ were not used in the statistical evaluation.

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

The assigned value is determined by consensus based on the test results oof 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, e.g. ISO or ASTM reproducibilities, the z-scores were calculated using a target standard deviation. This results in an evaluation independent of the variation of this interlaboratory study.

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

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

$z_{(target)}$ = (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

In this proficiency test some problems were encountered with the dispatch due to problems with custom clearance. The reporting time on the data entry portal was extended with another week. Four participants did not report any test result. All reporting participants reported before the extended reporting date.
In total 22 participants reported 222 numerical test results. Observed were 5 outlying test results, which is 2.3%. In proficiency studies, outlier percentages of 3% - 7.5% are quite normal.

Not all 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. 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 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 results tables of appendix 1 only the method number (sub) and year of adoption or revision e.g. D1209:05 will be used.

Acidity as Acetic acid: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D1613:17.

Aldehydes: Three participants reported the test as pass in accordance to ASTM D329:07(2021), which describes a pass/fail test. One other participant reported a numerical test result.

Appearance: This determination was not problematic. All reporting laboratories agreed on a test result of Pass (Bright & Clear).

Inorganic Chloride as Cl: This determination was not problematic. The reporting participants agreed on a value near or below the application range. Therefore, no z-scores are calculated.

Color Pt/Co: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D1209:05(2019).

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.

Specific Gravity 20/20°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 not problematic. One statistical outlier was observed. All three calculated reproducibilities (IBP, 50%recovered and DP) are in agreement with the requirements of ASTM D1078:11(2019) for automated and manual modes.

Miscibility with water (Hydrocarbons): This determination was not problematic. All reporting laboratories agreed on a test result of Pass.

Nonvolatile matter: This determination was not problematic. The reporting participants agreed on a value near or below the application range. Therefore, no z-scores are calculated.

Permanganate Time Test at 25°C: This determination may not problematic. All participants agreed on test result above 30 minutes. Therefore, no z-scores were calculated.

Purity by GC on dry basis: In this determination one statistical outlier was observed. The calculated reproducibility is higher than the calculated reproducibility of the 2019 PT iis19C11(0.025 %MM vs 0.018 %M/M).
This may be partly explained by rounding the test results to two decimals by the majority of the participants.

Diacetone alcohol: 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.

Mesityloxide: This determination was not problematic. The reporting participants agreed on a value near or below the application range. Therefore, no z-scores are calculated.

Methanol: This determination was not problematic. Two statistical outliers were observed. The calculated reproducibility after rejection of the statistical outliers is in agreement with the estimated reproducibility calculated with the Horwitz equation.

Refractive index at 20°C: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D1218:12(2016).

Water: 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 E203:16.

4.2 PERFORMANCE EVALUATION FOR THE GROUP OF LABORATORIES

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

Parameter	unit	n	average	2.8 * sd	R(lit)
Acidity as Acetic acid	mg/kg	20	14.3	10.1	14
Aldehydes		3	Pass	n.a.	n.a.
Appearance		20	Pass	n.a.	n.a.
Inorganic Chloride as Cl	mg/kg	6	<1	n.e.	n.e.
Color Pt/Co		16	2.8	3.3	7
Density at 20°C	kg/L	21	0.7905	0.0002	0.0005
Specific Gravity 20/20°C		18	0.7919	0.0001	0.0005
Initial Boiling Point	°C	19	55.9	0.3	0.9
50% recovered	°C	17	56.1	0.3	0.4
Dry Point	°C	19	56.3	0.5	0.6

Parameter	unit	n	average	2.8 * sd	R(lit)
Miscibility with water (Hydrocarb)		18	Pass	n.a.	n.a.
Nonvolatile matter	mg/100 mL	16	<1	n.e.	n.e.
Permanganate Time Test at 25°C	minutes	18	>30	n.e.	n.e.
Purity by GC on dry basis	%M/M	17	99.962	0.025	n.a.
Diacetone alcohol	mg/kg	12	5.9	2.9	2.0
Mesityloxide	mg/kg	14	<10	n.e.	n.e.
Methanol	mg/kg	15	255	45	50
Refractive Index at 20°C		16	1.3587	0.0004	0.0005
Water	%M/M	16	0.20	0.05	0.08

Table 3: Reproducibilities of tests on sample #21165

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

4.3 COMPARISON OF THE PROFICIENCY TEST OF SEPTEMBER 2021 WITH PREVIOUS PTS

	September 2021	September 2019	September 2017	September 2015	September 2013
Number of reporting laboratories	22	24	21	21	21
Number of test results	222	256	246	250	273
Number of statistical outliers	5	1	17	10	7
Percentage of statistical outliers	2.3%	0.4%	6.9%	4.0%	2.6%

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

Determination	September 2021	September 2019	September 2017	September 2015	September 2013
Acidity as Acetic acid	+	+	++	++	++
Inorganic Chloride as Cl	n.e.	n.e.	n.e.	n.e.	n.e.
Color Pt/Co	++	++	++	++	++
Density at 20°C	++	++	++	++	++
Specific Gravity 20/20°C	++	++	++	++	+
Distillation	+	+	++	++	++
Nonvolatile matter	n.e.	n.e.	(--)	(--)	++
Permanganate Time Test 25°C	n.e.	n.e.	(--)	(--)	(--)
Diacetone alcohol	-	(-)	(--)	(-)	(--)
Mesityloxide	n.e.	n.e.	--	-	+/-
Methanol	+/-	--	--	--	-
Refractive Index at 20°C	+	+/-	+	+/-	+

Determination	September 2021	September 2019	September 2017	September 2015	September 2013
Water	+	++	-	-	+/-

Table 5: comparison determinations against the reference test methods

Results between brackets should be used with due care.

The following performance categories were used:

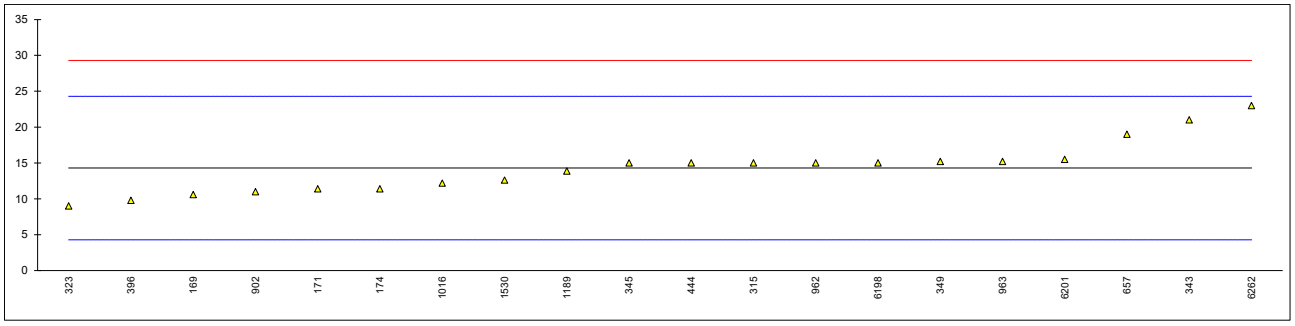
- ++ : group performed much better than the reference test method
- + : group performed better than the reference test method
- +/- : group performance equals the reference test method
- - : group performed worse than the reference test method
- -- : group performed much worse than the reference test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

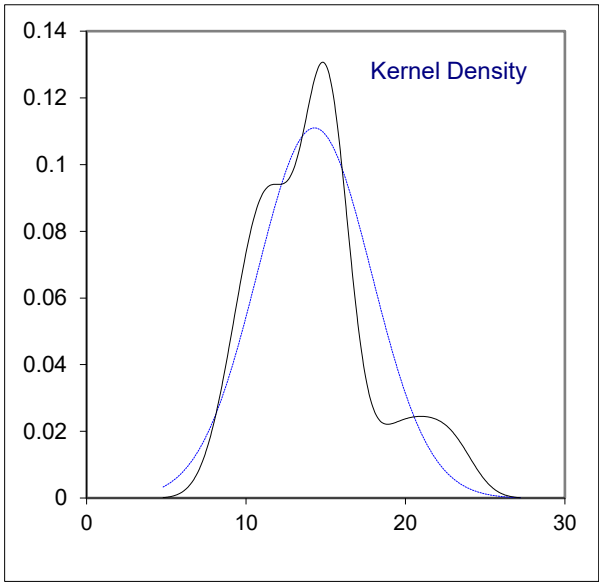
APPENDIX 1

Determination of Acidity as Acetic acid on sample #21165; results in mg/kg

lab	method	value	mark	z(targ)	remarks
169	D1613	10.6	C	-0.74	first reported 0.00106
171	D1613	11.4		-0.58	
174	D1613	11.4		-0.58	
315	D1613	15		0.14	
323	D1613	9		-1.06	
343	D1613	21		1.34	
345	D1613	15		0.14	
349	D1613	15.2	C	0.18	first reported 0.00152
396	D1613	9.8		-0.90	
444	D1613	15		0.14	
551		-----		-----	
557		-----		-----	
657	D1613	19		0.94	
886		-----		-----	
902	D1613	11		-0.66	
913		-----		-----	
962	D1613	15		0.14	
963	D1613	15.2		0.18	
1016	D1613	12.19		-0.42	
1189	D1613	13.88		-0.08	
1429		-----		-----	
1467		-----		-----	
1530	D1613	12.6		-0.34	
6198	D1613	15		0.14	
6201	D1613	15.5	C	0.24	first reported 0.0015
6262	D1613	23		1.74	

normality	OK
n	20
outliers	0
mean (n)	14.288
st.dev. (n)	3.5941
R(calc.)	10.064
st.dev.(D1613:17)	5
R(D1613:17)	14





Determination of Aldehydes on sample #21165;

lab	method	value	mark	z(targ)	remarks
169	D329	Pass		-----	
171		-----		-----	
174		-----		-----	
315		-----		-----	
323	D329	pass		-----	
343	D329	PASS		-----	
345	INH-023	32		-----	
349		-----		-----	
396		-----		-----	
444		-----		-----	
551		-----		-----	
557		-----		-----	
657		-----		-----	
886		-----		-----	
902		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016		-----		-----	
1189		-----		-----	
1429		-----		-----	
1467		-----		-----	
1530		-----		-----	
6198		-----		-----	
6201		-----		-----	
6262		-----		-----	
	n	3			
	Mean (n)	Pass			

Determination of Appearance on sample #21165;

lab	method	value	mark	z(targ)	remarks
169	E2680	CB&FSM		-----	
171	E2680	Pass		-----	
174	Visual	Clear and Free		-----	
315	E2680	pass		-----	
323	Visual	clear & bright liquid		-----	
343	INH-1608	C&B		-----	
345	D4176	Clear and bright		-----	
349	E2680	PASS		-----	
396	Visual	Clear and Bright		-----	
444	E2680	Pass		-----	
551		-----		-----	
557		-----		-----	
657	E2680	Pass		-----	
886		-----		-----	
902	E2680	PASS		-----	
913		-----		-----	
962	D4176	Clear & Bright		-----	
963	E2680	Pass		-----	
1016	Visual	Pass		-----	
1189	D4176	Br & Cl		-----	
1429		-----		-----	
1467		-----		-----	
1530	Visual	C & b		-----	
6198	D4176	pass		-----	
6201	D4176	Br & Cl		-----	
6262	Visual	Cl. & Br.		-----	
	n	20			
	mean (n)	Pass (Clear & Bright)			

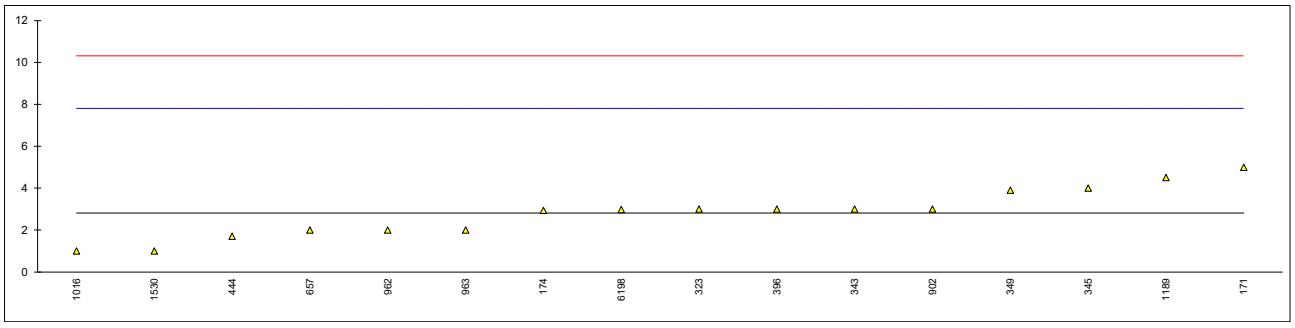
Determination of Inorganic Chloride as Cl on sample #21165; results in mg/kg

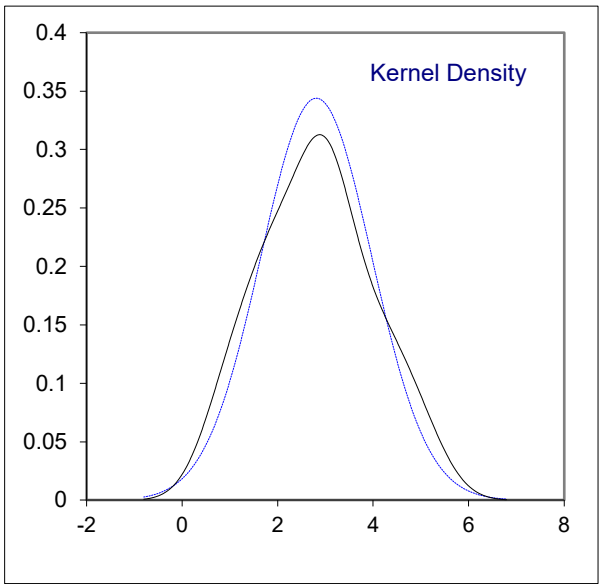
lab	method	value	mark	z(targ)	remarks
169		-----		-----	
171	IMPCA002	<0.25		-----	
174		-----		-----	
315	INH-158	<0.2		-----	
323	INH-008	<1		-----	
343		-----		-----	
345		-----		-----	
349		-----		-----	
396		-----		-----	
444		-----		-----	
551		-----		-----	
557		-----		-----	
657		-----		-----	
886		-----		-----	
902		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016		-----		-----	
1189	IMPCA002	0.003		-----	
1429	ISO6227	<1		-----	
1467		-----		-----	
1530		-----		-----	
6198		-----		-----	
6201	IMPCA002	0.03		-----	
6262		-----		-----	
	outliers	6			
	mean (n)	<1			

Determination of Color Pt/Co on sample #21165;

lab	method	value	mark	z(targ)	remarks
169	D1209	<5		-----	
171	D1209	5		0.87	
174	D5386	2.94		0.05	
315	D1209	<5		-----	
323	D1209	3		0.07	
343	D1209	3		0.07	
345	D1209	4		0.47	
349	D5386	3.9		0.43	
396	D1209	3		0.07	
444	D5386	1.7		-0.45	
551		-----		-----	
557		-----		-----	
657	D1209	2		-0.33	
886	D1209	<5		-----	
902	D5386	3		0.07	
913		-----		-----	
962	D1209	2		-0.33	
963	D1209	2		-0.33	
1016	D1209	1		-0.73	
1189	D1209	4.5		0.67	
1429	D1209	<5		-----	
1467		-----		-----	
1530	D1209	1		-0.73	
6198	D5386	2.98		0.07	
6201	D1209	<5		-----	
6262	D1209	<5		-----	

normality	OK
n	16
outliers	0
mean (n)	2.81
st.dev. (n)	1.160
R(calc.)	3.25
st.dev.(D1209:05)	2.5
R(D1209:05)	7

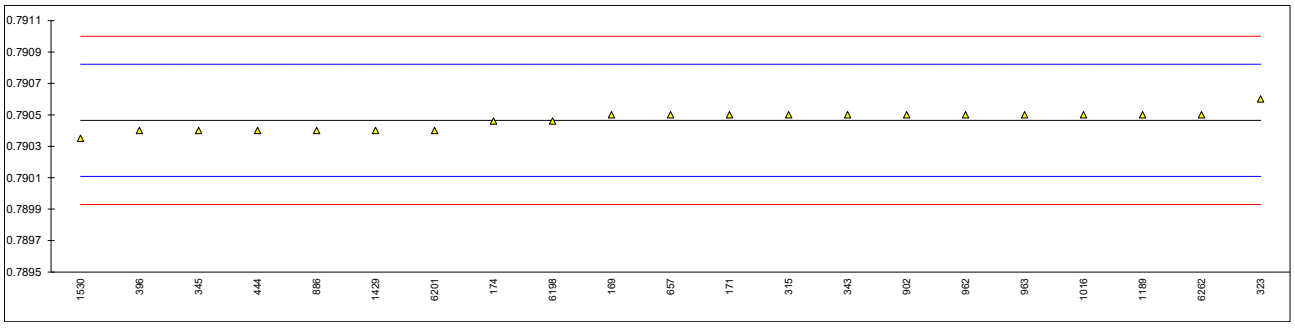


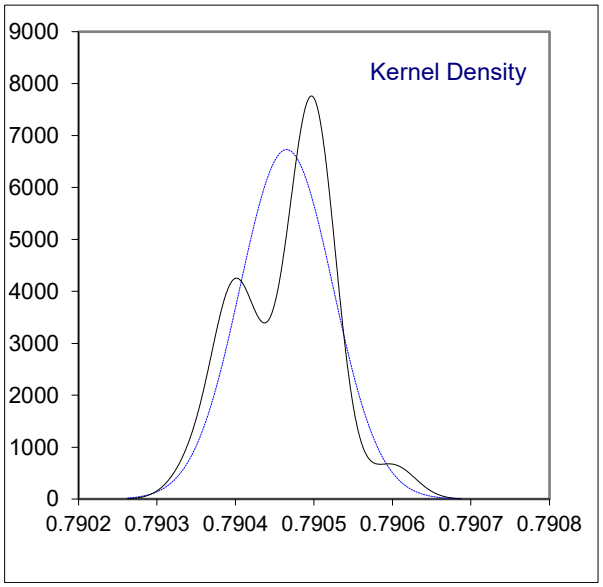


Determination of Density at 20°C on sample #21165; results in kg/L

lab	method	value	mark	z(targ)	remarks
169	D4052	0.7905		0.20	
171	D4052	0.7905		0.20	
174	D4052	0.79046		-0.03	
315	D4052	0.7905		0.20	
323	D4052	0.7906		0.76	
343	D4052	0.7905		0.20	
345	D4052	0.7904		-0.36	
349		-----		-----	
396	D4052	0.7904		-0.36	
444	D4052	0.7904		-0.36	
551		-----		-----	
557		-----		-----	
657	D4052	0.7905		0.20	
886	D4052	0.7904		-0.36	
902	D4052	0.7905		0.20	
913		-----		-----	
962	D4052	0.7905		0.20	
963	ISO12185	0.7905		0.20	
1016	ISO12185	0.7905		0.20	
1189	ISO12185	0.7905		0.20	
1429	D4052	0.7904		-0.36	
1467		-----		-----	
1530	ISO12185	0.79035		-0.64	
6198	D4052	0.79046		-0.03	
6201	ISO12185	0.7904	C	-0.36	first reported 790.4
6262	ISO12185	0.7905		0.20	

normality	OK
n	21
outliers	0
mean (n)	0.79047
st.dev. (n)	0.000059
R(calc.)	0.00017
st.dev.(ISO12185:96)	0.000179
R(ISO12185:96)	0.0005

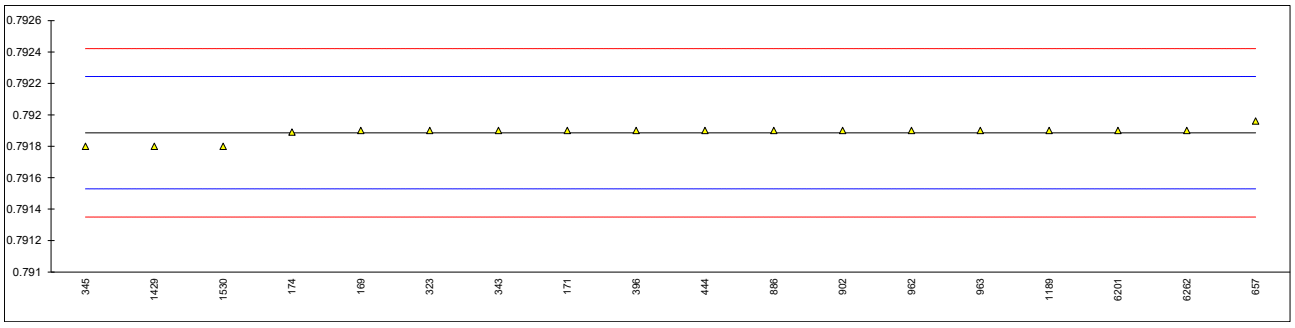


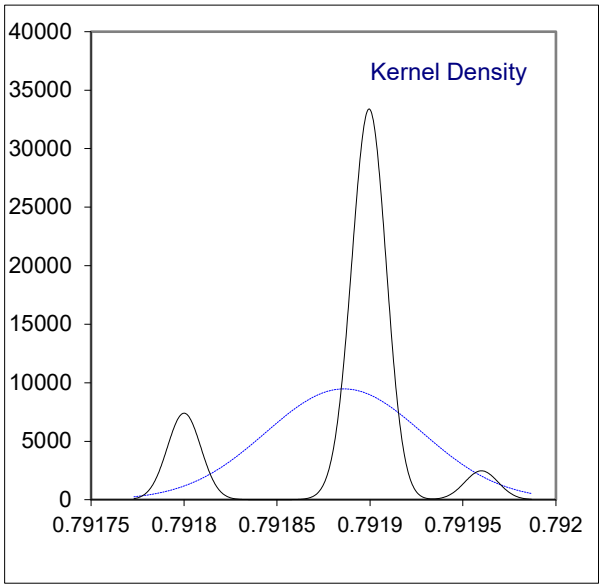


Determination of Specific Gravity 20/20°C on sample #21165;

lab	method	value	mark	z(targ)	remarks
169	D4052	0.7919		0.08	
171	D4052	0.7919		0.08	
174	D4052	0.79189		0.02	
315		-----		-----	
323	D4052	0.7919		0.08	
343	D4052	0.7919		0.08	
345	D4052	0.7918		-0.48	
349		-----		-----	
396	D4052	0.7919		0.08	
444	D4052	0.7919		0.08	
551		-----		-----	
557		-----		-----	
657	D4052	0.79196		0.41	
886	D4052	0.7919		0.08	
902	D4052	0.7919		0.08	
913		-----		-----	
962	D4052	0.7919		0.08	
963	ISO12185	0.7919		0.08	
1016		-----		-----	
1189	ISO12185	0.7919		0.08	
1429	D4052	0.7918		-0.48	
1467		-----		-----	
1530	D4052	0.79180		-0.48	
6198		-----		-----	
6201	ISO12185	0.7919	C	0.08	first reported 791.9
6262	ISO12185	0.7919		0.08	

normality	suspect
n	18
outliers	0
mean (n)	0.79189
st.dev. (n)	0.000042
R(calc.)	0.00012
st.dev.(ISO12185:96)	0.000179
R(ISO12185:96)	0.0005

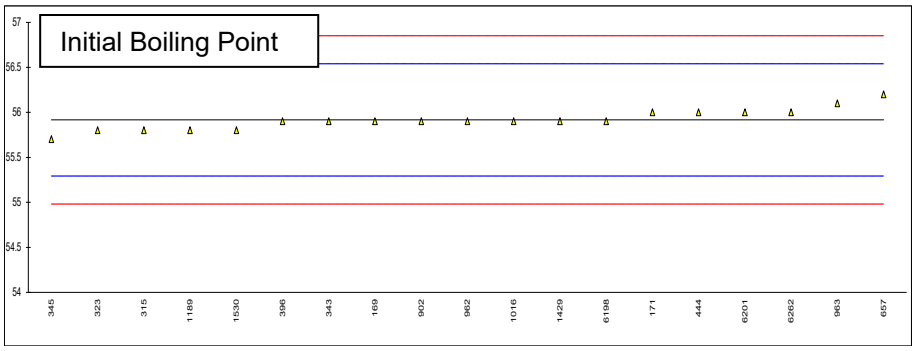


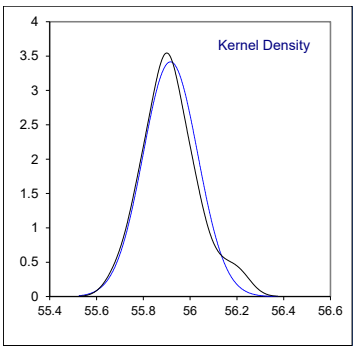


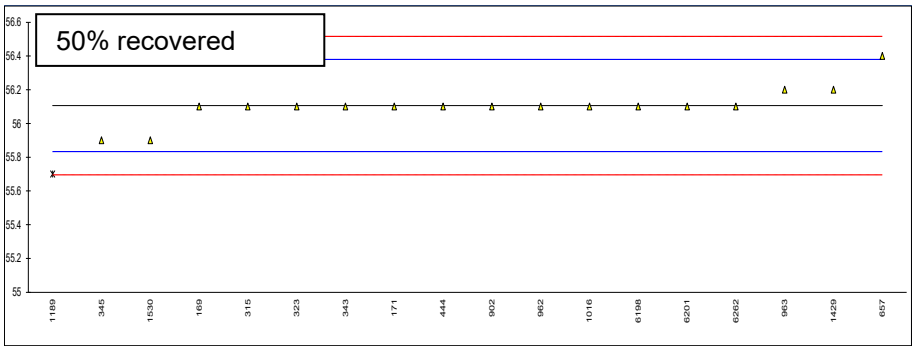
Determination of Initial Boiling point, 50% recovered and Dry Point on sample #21165; results in °C

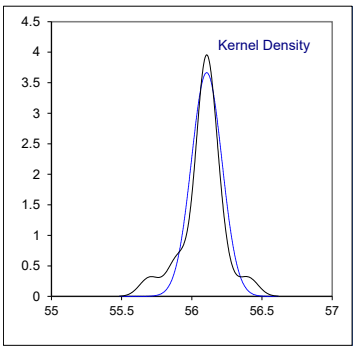
lab	method	IBP	mark	z(targ)	50% rec.	mark	z(targ)	DP	mark	z(targ)	range
169	D1078-automated	55.9		-0.05	56.1		-0.04	56.3		0.10	0.4
171	D1078-automated	56.0		0.27	56.1		-0.04	56.7		1.96	0.7
174		-----		-----	-----		-----	-----		-----	-----
315	D1078-automated	55.8		-0.37	56.1		-0.04	56.2		-0.37	0.4
323	D1078-automated	55.8		-0.37	56.1		-0.04	56.2		-0.37	0.4
343	D1078-automated	55.9		-0.05	56.1		-0.04	56.2		-0.37	0.3
345	D1078-automated	55.7		-0.69	55.9		-1.50	56.1		-0.83	0.4
349		-----		-----	-----		-----	-----		-----	-----
396	D1078-manual	55.9		-0.05	-----		-----	56.4		0.56	0.5
444	D1078-automated	56.0		0.27	56.1		-0.04	56.3		0.10	0.3
551		-----		-----	-----		-----	-----		-----	-----
557		-----		-----	-----		-----	-----		-----	-----
657	D1078-automated	56.2		0.91	56.4		2.15	56.4	C	0.56	0.5
886		-----		-----	-----		-----	-----		-----	-----
902	D1078-automated	55.9		-0.05	56.1		-0.04	56.4		0.56	0.5
913		-----		-----	-----		-----	-----		-----	-----
962	D1078-automated	55.9		-0.05	56.1		-0.04	56.3		0.10	0.4
963		56.1		0.59	56.2		0.69	56.4		0.56	0.3
1016	D1078-automated	55.9		-0.05	56.1		-0.04	56.3		0.10	-----
1189	D1078-automated	55.8	C	-0.37	55.7	G(0.05)	-2.97	55.9		-1.76	0.5
1429	D1078-automated	55.9		-0.05	56.2		0.69	56.3		0.10	0.4
1467		-----		-----	-----		-----	-----		-----	-----
1530	D1078-automated	55.80		-0.37	55.90		-1.50	56.10		-0.83	0.30
6198	D1078-automated	55.9		-0.05	56.1		-0.04	56.3		0.10	0.5
6201	D1078-automated	56.0		0.27	56.1		-0.04	56.3		0.10	0.3
6262	D1078-automated	56.0		0.27	56.1		-0.04	56.2		-0.37	0.2
	normality	OK			not OK			not OK			
	n	19			17			19			
	outliers	0			1			0			
	mean (n)	55.92			56.11			56.28			
	st.dev. (n)	0.117			0.109			0.162			
	R(calc.)	0.33			0.30			0.45			
	st.dev.(D1078-A:11)	0.312			0.137			0.215			
	R(D1078-A:11)	0.87			0.38			0.60			
Compare											
	R(D1078-M:11)	0.60			0.36			0.73			

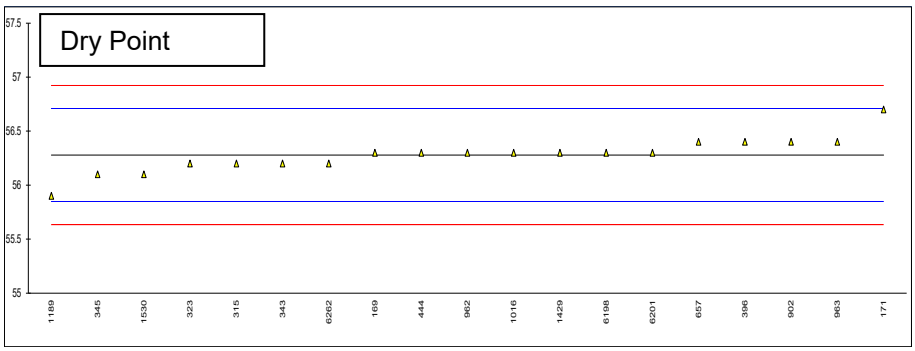
lab 1189 first reported 55.4
lab 657 first reported 56.7

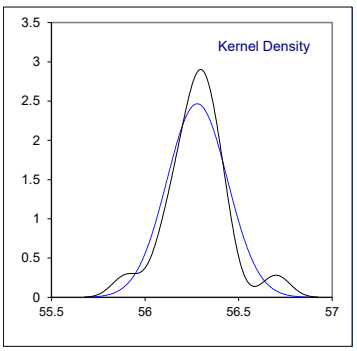

Initial Boiling Point


Kernel Density


50% recovered


Kernel Density


Dry Point


Kernel Density

Determination of Miscibility with water (Hydrocarbons) on sample #21165;

lab	method	value	mark	z(targ)	remarks
169	D1722	Pass		-----	
171	D1722	Pass		-----	
174	D1722	Pass		-----	
315	D1722	pass		-----	
323	D1722	pass		-----	
343		-----		-----	
345	D1722	Passes test		-----	
349		-----		-----	
396	D1722	Passed Test		-----	
444	D1722	Pass		-----	
551		-----		-----	
557		-----		-----	
657	D1722	Pass		-----	
886		-----		-----	
902	D1722	PASS		-----	
913		-----		-----	
962	D1722	Pass		-----	
963	D1722	Pass		-----	
1016	D1722	Pass		-----	
1189	D1722	pass		-----	
1429		-----		-----	
1467		-----		-----	
1530	D1722	pass		-----	
6198	D1722	pass		-----	
6201	D1722	pass		-----	
6262	D1722	Passed		-----	
	n	18			
	mean (n)	Pass			

Determination of Nonvolatile matter on sample #21165; results in mg/100 mL

lab	method	value	mark	z(targ)	remarks
169	D1353	0.0		-----	
171	D1353	<1		-----	
174		-----		-----	
315	D1353	<1		-----	
323	D1353	<1		-----	
343	D1353	<0,1		-----	
345	D1353	<0.1		-----	
349		-----		-----	
396	D1353	<1		-----	
444	D1353	0		-----	
551		-----		-----	
557		-----		-----	
657	D1353	<1		-----	
886		-----		-----	
902		-----		-----	
913		-----		-----	
962	D1353	0.8		-----	
963	D1353	0.8		-----	
1016	D1353	0.3		-----	
1189	D1353	< 0.01		-----	
1429		-----		-----	
1467		-----		-----	
1530		-----		-----	
6198	D1353	<0.001		-----	
6201	D1353	<1		-----	
6262	D1353	<1		-----	
	n	16			
	mean (n)	<1			

Determination of Permanganate Time Test at 25°C on sample #21165; results in minutes

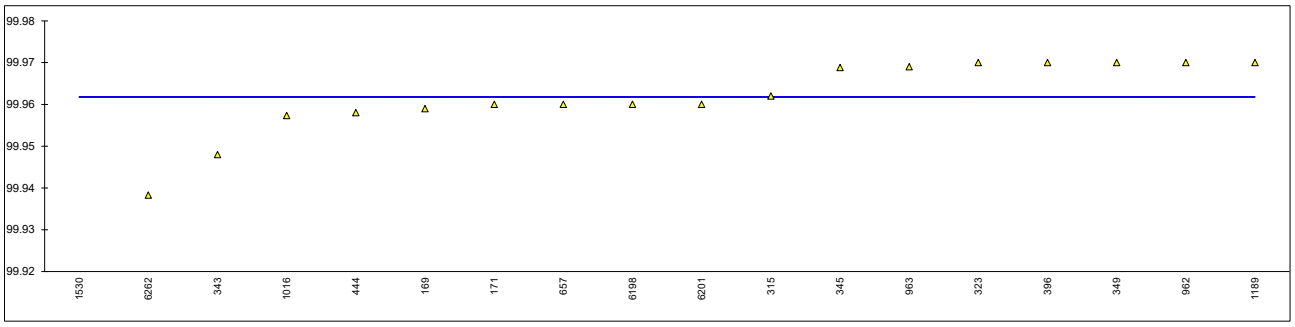
lab	method	value	mark	z(targ)	remarks
169	D1363	>120		-----	
171	D1363	>120		-----	
174	D1363	>120		-----	
315	D1363	>240		-----	
323	D1363	>30		-----	
343	D1363	>150		-----	
345	D1363	>30		-----	
349		-----		-----	
396	D1363	>150		-----	
444	D1363	>180		-----	
551		-----		-----	
557		-----		-----	
657	D1363	>30		-----	
886		-----		-----	
902	D1363	>30		-----	
913		-----		-----	
962	D1363	>30		-----	
963	D1363	>30		-----	
1016	D1363	>300		-----	
1189	D1363	>240		-----	
1429		-----		-----	
1467		-----		-----	
1530		-----		-----	
6198	D1363	>120		-----	
6201	D1363	>30		-----	
6262	D1363	>30		-----	
	n	18			
	mean (n)	>30			

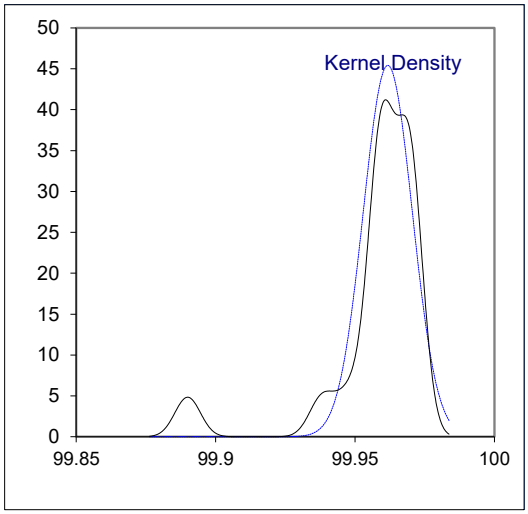
Determination of Purity by GC on dry basis on sample #21165, results in %M/M

lab	method	value	mark	z(targ)	remarks
169	INH-ACS	99.959		-----	
171	INH-001	99.96		-----	
174		-----		-----	
315	INH-394	99.962		-----	
323	INH-020	99.97		-----	
343	INH-4011	99.9480		-----	
345	INH-023	99.9688		-----	
349	INH-034	99.97		-----	
396	D7504	99.97		-----	
444	INH-020	99.958		-----	
551		-----		-----	
557		-----		-----	
657	INH-009	99.96		-----	
886		-----		-----	
902		-----		-----	
913		-----		-----	
962	INH-012	99.97		-----	
963	INH-012	99.969		-----	
1016	DIN55687	99.9573184		-----	
1189	In house	99.97		-----	
1429		-----		-----	
1467		-----		-----	
1530	Ph.Eur. 2.2.28	99.89	G(0.01)	-----	
6198	GB/T6026/D329	99.96		-----	
6201	In house	99.96		-----	
6262	ISO6353-2	99.9383		-----	

normality	suspect
n	17
outliers	1
mean (n)	99.962
st.dev. (n)	0.0088
R(calc.)	0.025
st.dev.(lit)	unknown
R(lit)	unknown

Compare R(iis19C11) = 0.01764

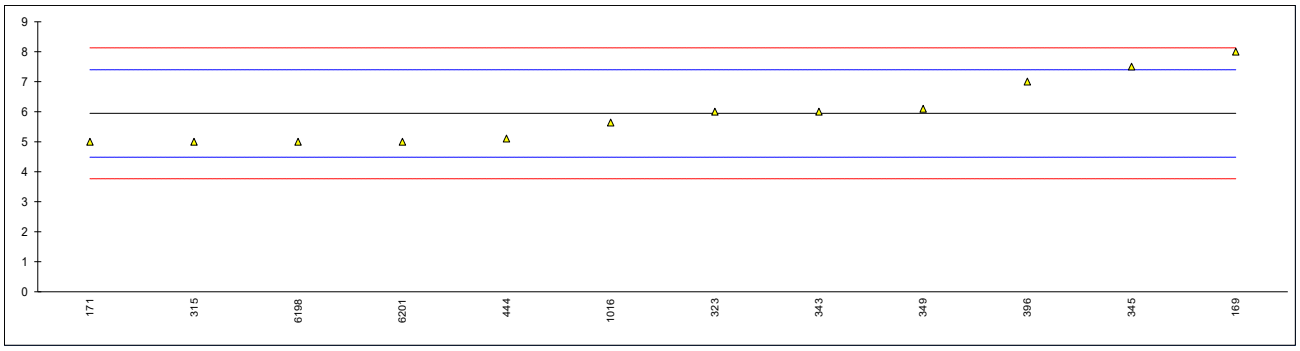


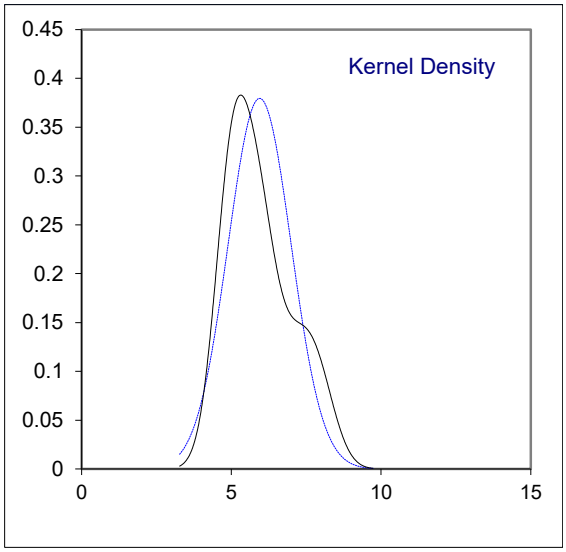


Determination of Diacetone alcohol on sample #21165, results in mg/kg

lab	method	value	mark	z(targ)	remarks
169	INH-ACS	8	C	2.83	first reported 0
171	INH-001	5		-1.30	
174		-----		-----	
315	INH-394	5		-1.30	
323	INH-020	6		0.08	
343	INH-4714	6		0.08	
345	INH-023	7.5		2.14	
349	INH-034	6.1		0.21	
396	D7504	7		1.45	
444	INH-020	5.1		-1.16	
551		-----		-----	
557		-----		-----	
657	INH-009	<5		-----	
886		-----		-----	
902		-----		-----	
913		-----		-----	
962	INH-012	<5		-----	
963		-----		-----	
1016	DIN55687	5.635		-0.43	
1189		-----	W	-----	test result withdrawn, first reported < 0.1
1429		-----		-----	
1467		-----		-----	
1530		-----		-----	
6198	GB/T6026/D329	5		-1.30	
6201	In house	5		-1.30	
6262	ISO6353-2	<5	C	-----	first reported 12

normality	OK
n	12
outliers	0
mean (n)	5.945
st.dev. (n)	1.0517
R(calc.)	2.945
st.dev.(Horwitz)	0.7273
R(Horwitz)	2.036





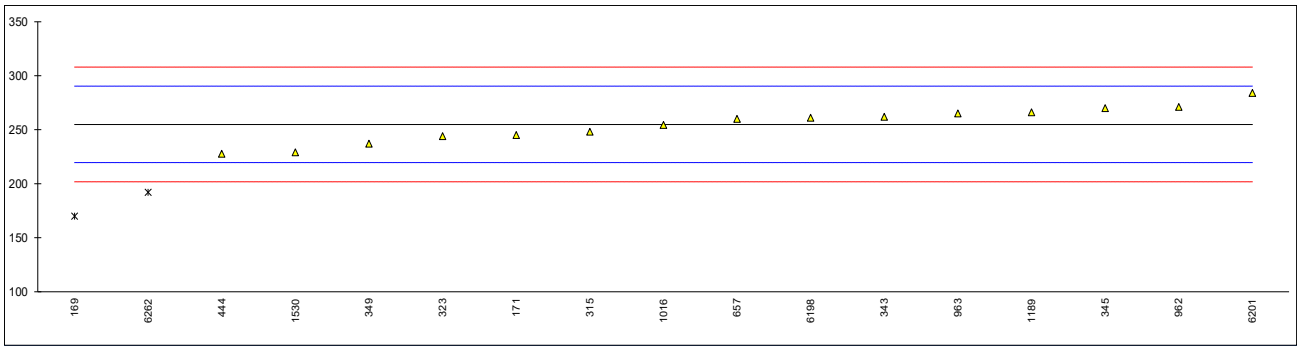
Determination of Mesityloxide on sample #21165, results in mg/kg

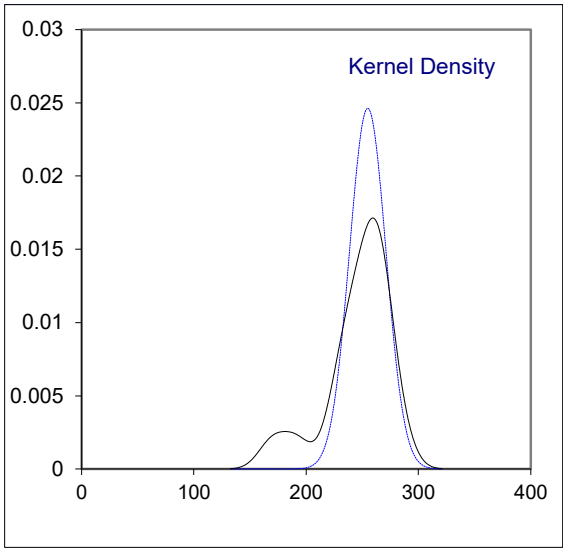
lab	method	value	mark	z(targ)	remarks
169		-----		-----	
171		-----		-----	
174		-----		-----	
315	INH-394	<1		-----	
323	INH-020	<5		-----	
343	INH-4714	0		-----	
345	INH-023	<1		-----	
349		-----		-----	
396	D7504	<2		-----	
444	INH-020	0		-----	
551		-----		-----	
557		-----		-----	
657	INH-009	<5		-----	
886		-----		-----	
902		-----		-----	
913		-----		-----	
962	INH-012	<5		-----	
963	INH-012	<10		-----	
1016	DIN55687	0		-----	
1189	In house	<0.1		-----	
1429		-----		-----	
1467		-----		-----	
1530		-----		-----	
6198	GB/T6026/D329	<1		-----	
6201	In house	<1		-----	
6262	ISO6353-2	<10		-----	
	n	14			
	mean (n)	<10			

Determination of Methanol on sample #21165, results in mg/kg

lab	method	value	mark	z(targ)	remarks
169	INH-ACS	170	C,DG(0.01)	-4.79	first reported 165
171	INH-001	245		-0.56	
174		-----		-----	
315	INH-394	248		-0.39	
323	INH-020	244		-0.62	
343	INH-4714	262		0.40	
345	INH-023	270		0.85	
349	INH-034	237		-1.01	
396		-----		-----	
444	INH-020	227.6		-1.54	
551		-----		-----	
557		-----		-----	
657	INH-009	260		0.29	
886		-----		-----	
902		-----		-----	
913		-----		-----	
962	INH-012	271		0.91	
963	INH-012	265		0.57	
1016	DIN55687	254.428		-0.03	
1189	In house	266		0.62	
1429		-----		-----	
1467		-----		-----	
1530	Ph.Eur. 2.2.28	229		-1.46	
6198	GB/T6026/D329	261		0.34	
6201	In house	284		1.64	
6262	ISO6353-2	192	C,DG(0.01)	-3.55	first reported 373

normality	OK
n	15
outliers	2
mean (n)	254.94
st.dev. (n)	16.200
R(calc.)	45.36
st.dev.(Horwitz)	17.715
R(Horwitz)	49.60

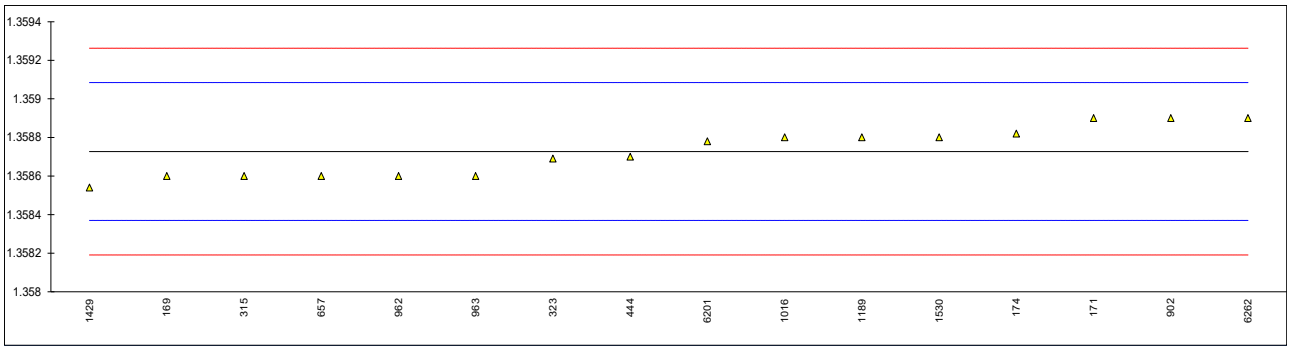


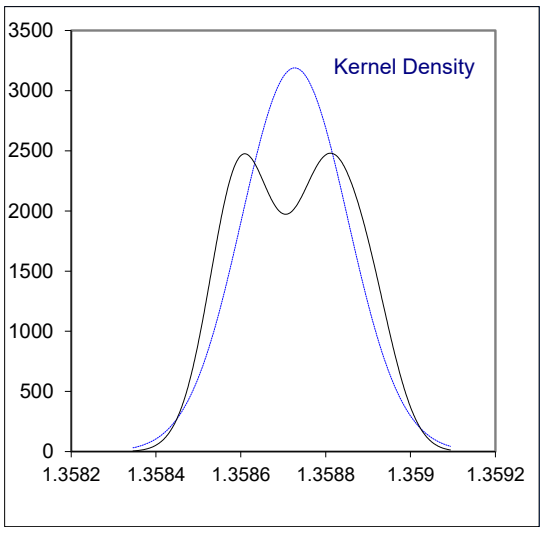


Determination of Refractive Index at 20°C on sample #21165;

lab	method	value	mark	z(targ)	remarks
169	D1218	1.3586		-0.71	
171	D1218	1.3589		0.97	
174	D1218	1.35882		0.52	
315	D1218	1.3586		-0.71	
323	D1218	1.35869		-0.21	
343		-----		-----	
345		-----		-----	
349		-----		-----	
396		-----		-----	
444	D1218	1.3587		-0.15	
551		-----		-----	
557		-----		-----	
657	D1218	1.3586		-0.71	
886		-----		-----	
902	D1218	1.3589		0.97	
913		-----		-----	
962	D1218	1.3586		-0.71	
963	D1218	1.35860		-0.71	
1016	D1218	1.3588		0.41	
1189	D1218	1.3588	C	0.41	first reported 1.3595
1429	D1218	1.35854		-1.05	
1467		-----		-----	
1530	D1218	1.3588		0.41	
6198		-----		-----	
6201	D1218	1.35878		0.30	
6262	D1218	1.3589		0.97	

normality	OK
n	16
outliers	0
mean (n)	1.35873
st.dev. (n)	0.000125
R(calc.)	0.00035
st.dev.(D1218:12)	0.000179
R(D1218:12)	0.0005

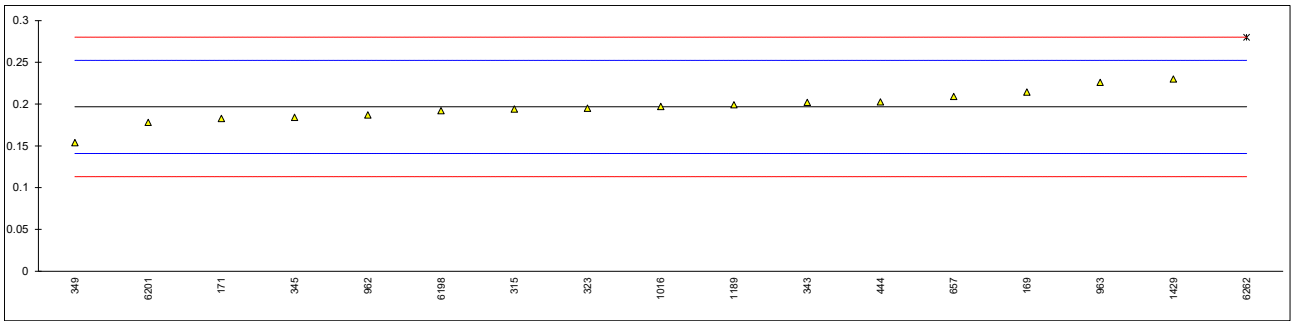


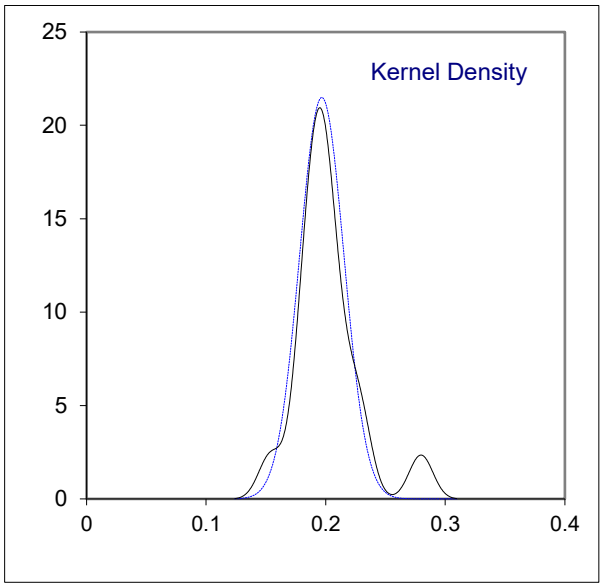


Determination of Water on sample #21165; results in %M/M

lab	method	value	mark	z(targ)	remarks
169	E203	0.2143	C	0.63	first reported 0.2568
171	E203	0.1828		-0.50	
174		-----		-----	
315	E203	0.194		-0.10	
323	E203	0.195		-0.06	
343	E203	0.202		0.19	
345	D1364	0.184		-0.45	
349	D1364	0.1538	C	-1.54	first reported 1538
396		-----		-----	
444	E203	0.2026		0.21	
551		-----		-----	
557		-----		-----	
657	E203	0.209		0.44	
886		-----		-----	
902		-----		-----	
913		-----		-----	
962	E203	0.187		-0.35	
963	E203	0.2260		1.05	
1016	D1364	0.197		0.01	
1189	D1364	0.199		0.08	
1429	E203	0.23		1.20	
1467		-----		-----	
1530		-----		-----	
6198	D1364	0.192		-0.17	
6201	E203	0.178		-0.67	
6262	E203	0.2797	G(0.01)	2.98	

normality	suspect
n	16
outliers	1
mean (n)	0.19666
st.dev. (n)	0.018561
R(calc.)	0.05197
st.dev.(E203:16)	0.027857
R(E203:16)	0.078





APPENDIX 2

Number of participants per country

2 labs in BELGIUM
2 labs in BRAZIL
1 lab in CHINA, People's Republic
1 lab in GERMANY
1 lab in INDIA
1 lab in ITALY
4 labs in NETHERLANDS
3 labs in SAUDI ARABIA
1 lab in SINGAPORE
3 labs in SPAIN
1 lab in TAIWAN
1 lab in TURKEY
2 labs in UNITED KINGDOM
3 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

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