Institute for
Interlaboratory Studies

Results of Proficiency Test
Acetone
September 2023

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 based on the latest version of ASTM D329 once every two years. During the annual proficiency testing program of 2023 it was decided to continue the round robin for the analysis of Acetone.

In this interlaboratory study 24 laboratories in 14 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 a laboratory that has performed the tests in accordance with for ISO/IEC17043 relevant requirements of ISO/IEC17025.
It was decided to send a one sample Acetone in a 1-liter amber glass bottle labelled #23165.
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 of Acetone was obtained from a local supplier. After homogenization 35 amber glass bottles of 1 L were filled and labelled #23165.
The homogeneity of the subsamples was checked by determination of Density at 20 °C in accordance with D4052 and Water in accordance with ASTM E203 on 4 stratified randomly selected subsamples.

	Density at 20 °C in kg/L	Water in mg/kg
sample #23165-1	0.79050	2250
sample #23165-2	0.79052	2300
sample #23165-3	0.79051	2210
sample #23165-4	0.79052	2250

Table 1: homogeneity test results of subsamples #23165

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 mg/kg
r (observed)	0.00003	103
reference test method	ISO12185:96	ASTM E203:23
0.3 x R (reference test method)	0.00015	234

Table 2: evaluation of the repeatabilities of subsamples #23165

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 1 L bottle of Acetone labelled #23165 was sent on August 23, 2023. An SDS was added to the sample package.

2.5 STABILITY OF THE SAMPLES

The stability of Acetone 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: 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), Water miscibility (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 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.
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 of the samples. Therefore, the reporting time on the data entry portal was extended with another week. Three participants reported test results after the extended reporting date and six other participants did not report any test results. Not all participants were able to report all tests requested.
In total 18 participants reported 197 numerical test results. Observed were 11 outlying test results, which is 5.6%. In proficiency tests 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 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). When a method has been reapproved an “R” will be added and the year of approval (e.g. D1209:05R19).

Acidity as Acetic acid: The group of participants met the target requirements. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D1613:17R23.

Aldehydes: Two participants reported the test as pass in accordance with ASTM D329, which describes a pass/fail test. Two other participants reported a numerical test result.

Appearance: All reporting laboratories agreed on a test result of Pass (Clear & Bright).

Inorganic Chloride as Cl: The reporting participants agreed on a value near or below the level of detection. Therefore, no z-scores are calculated.

Color Pt/Co: The group of participants met the target requirements. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D1209:05R19.

Density at 20 °C: The group of participants met the target requirements. One statistical outlier was observed. The calculated reproducibility after rejection of the statistical outlier is in agreement with the requirements of ISO12185:96.

Specific Gravity 20/20 °C: The group of participants met the target requirements. One statistical outlier was observed. The calculated reproducibility after rejection of the statistical outlier is in agreement with the requirements of ISO12185:96.

Distillation: The group of participants met the target requirements. In total one statistical outlier was observed over three parameters. All three calculated reproducibilities (IBP, 50% recovered and DP) after rejection of the statistical outlier are in agreement with the requirements of ASTM D1078:11R19 for both automated and manual mode.

Water miscibility (Hydrocarbons): All reporting laboratories agreed on a test result of Pass.

Nonvolatile matter: Almost all reporting participants agreed on a value near or below the level of detection. Therefore, no z-scores are calculated.

Permanganate Time Test at 25 °C: 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. Regretfully, the methods used do not provide any reproducibility limit. Therefore, no z-scores were calculated.

Diacetone alcohol: The group of participants may have had difficulty to meet the target requirements. Two statistical outliers were observed. The calculated reproducibility after rejection of the statistical outliers is not in agreement with the estimated reproducibility calculated with the Horwitz equation.

Mesityloxide: The group of participants met the target requirements. Three 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.

Methanol: The group of participants may have had difficulty to meet the target requirements. One statistical outlier was observed. The calculated reproducibility after rejection of the statistical outlier is not in agreement with the estimated reproducibility calculated with the Horwitz equation.

Refractive index at 20 °C: The group of participants met the target requirements. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D1218:21.

Water: The group of participants met the target requirements. One statistical outlier was observed. The calculated reproducibility after rejection of the statistical outlier is in agreement with the requirements of ASTM E203:23.

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 methods are presented in the next table.

Parameter	unit	n	average	2.8 * sd	R(lit)
Acidity as Acetic acid	mg/kg	14	16.8	13.9	14
Aldehydes		2	Pass	n.a.	n.a.
Appearance		15	Pass (Cl&Br)	n.a.	n.a.
Inorganic Chloride as Cl	mg/kg	4	<1	n.e.	n.e.
Color Pt/Co		14	3.5	2.5	7
Density at 20 °C	kg/L	17	0.7905	0.0002	0.0005
Specific Gravity 20/20 °C		11	0.7920	0.0001	0.0005
Initial Boiling Point	°C	13	55.9	0.2	0.9
50% recovered	°C	14	56.1	0.2	0.4
Dry Point	°C	14	56.3	0.2	0.6
Water miscibility (Hydrocarbons)		14	Pass	n.a.	n.a.
Nonvolatile matter	mg/100 mL	10	<1	n.e.	n.e.
Permanganate Time Test at 25 °C	minutes	12	>30	n.e.	n.e.
Purity by GC on dry basis	%M/M	13	99.971	0.010	n.a.

Parameter	unit	n	average	2.8 * sd	R(lit)
Diacetone alcohol	mg/kg	12	116	45	25
Mesityloxide	mg/kg	9	33.5	3.6	8.9
Methanol	mg/kg	13	76.5	25.7	17.8
Refractive Index at 20 °C		11	1.3587	0.0003	0.0005
Water	mg/kg	15	2111	514	780

Table 3: reproducibilities of tests on sample #23165

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 2023 WITH PREVIOUS PTS

	September 2023	September 2021	September 2019	September 2017	September 2015
Number of reporting laboratories	18	22	24	21	21
Number of test results	197	222	256	246	250
Number of statistical outliers	11	5	1	17	10
Percentage of statistical outliers	5.6%	2.3%	0.4%	6.9%	4.0%

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 in the following table.

Determination	September 2023	September 2021	September 2019	September 2017	September 2015
Acidity as Acetic acid	+/-	+	+	++	++
Color Pt/Co	++	++	++	++	++
Density at 20 °C	++	++	++	++	++
Specific Gravity 20/20 °C	++	++	++	++	++
Distillation	++	+	+	++	++
Nonvolatile matter	n.e.	n.e.	n.e.	(--)	(--)
Permanganate Time Test 25 °C	n.e.	n.e.	n.e.	(--)	(--)
Diacetone alcohol	-	-	(-)	(--)	(-)
Mesityloxide	++	n.e.	n.e.	--	-
Methanol	-	+/-	--	--	--
Refractive Index at 20 °C	+	+	+/-	+	+/-
Water	+	+	++	-	-

Table 5: comparison of determinations to the reference test methods

For results between brackets no z-scores are calculated.

The following performance categories were used:

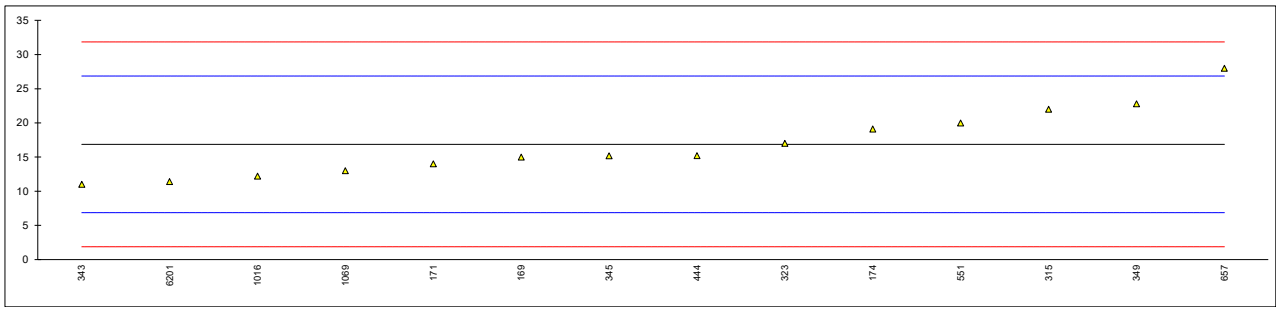
- ++ : group performed much better than the reference test method
- + : group performed better than the reference test method
- +/- : group performance equals the reference test method
- - : group performed worse than the reference test method
- -- : group performed much worse than the reference test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

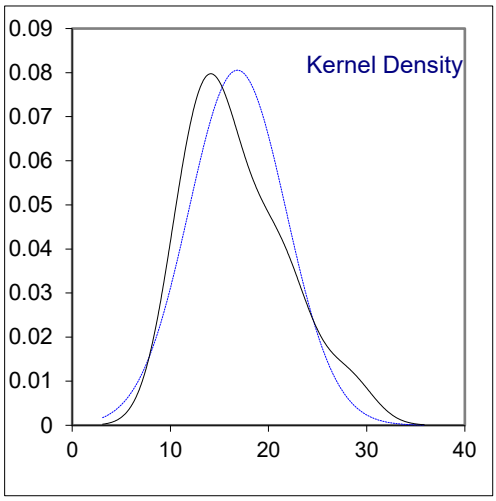
APPENDIX 1

Determination of Acidity as Acetic acid on sample #23165; results in mg/kg

Lab	method	value	mark	z(targ)	remarks
169	D1613	15		-0.37	
171	D1613	14		-0.57	
174	D1613	19.1		0.45	
315	D1613	22		1.03	
323	D1613	17		0.03	
343	D1613	11		-1.17	
345	D1613	15.18		-0.33	
349	D1613	22.8		1.19	
396		-----		-----	
444	D1613	15.2		-0.33	
551	D1613	20		0.63	
557		-----		-----	
657	D1613	28		2.23	
886		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016	D1613	12.2		-0.93	
1069	D1613	13		-0.77	
1429		-----		-----	
1530		-----		-----	
6198		-----		-----	
6201	D1613	11.4		-1.09	
6438		-----		-----	

normality	OK
n	14
outliers	0
mean (n)	16.849
st.dev. (n)	4.9512
R(calc.)	13.863
st.dev.(D1613:17R23)	5
R(D1613:17R23)	14





Determination of Aldehydes on sample #23165;

lab	method	value	mark	z(targ)	remarks
169	D329	passes test		-----	
171		-----		-----	
174		-----		-----	
315		-----		-----	
323	D329	<50		-----	
343	D329	Pass		-----	
345	INH-023	33		-----	
349		-----		-----	
396		-----		-----	
444		-----		-----	
551		-----		-----	
557		-----		-----	
657		-----		-----	
886		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016		-----		-----	
1069		-----		-----	
1429		-----		-----	
1530		-----		-----	
6198		-----		-----	
6201		-----		-----	
6438		-----		-----	
	n	2			
	mean (n)	Pass			

Determination of Appearance on sample #23165;

lab	method	value	mark	z(targ)	remarks
169	E2680	clear, bright, free from solid matter and undissol		-----	
171	E2680	Pass		-----	
174	Visual	Clear and Free		-----	
315	E2680	pass		-----	
323	INH-001	CFFMIS		-----	
343	E2680	Pass		-----	
345	D4176	clear and bright		-----	
349	E2680	pass		-----	
396	Visual	C&B		-----	
444	E2680	Pass		-----	
551	E2680	Pass		-----	
557		-----		-----	
657	E2680	Pass		-----	
886		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016	Visual	Clear and Bright, no particles		-----	
1069	Visual	bright & clear		-----	
1429		-----		-----	
1530		-----		-----	
6198		-----		-----	
6201	Visual	Cl &Br		-----	
6438		-----		-----	
	n	15			
	mean (n)	Pass (Clear and Bright)			

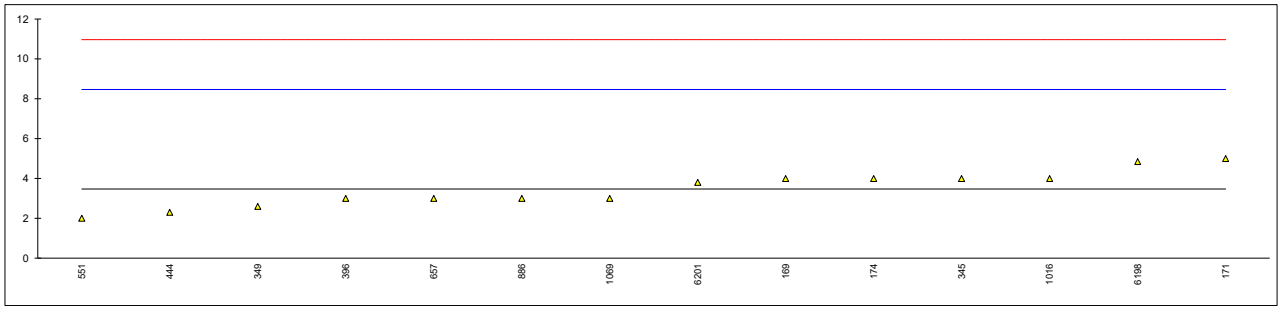
Determination of Inorganic Chloride as Cl on sample #23165; results in mg/kg

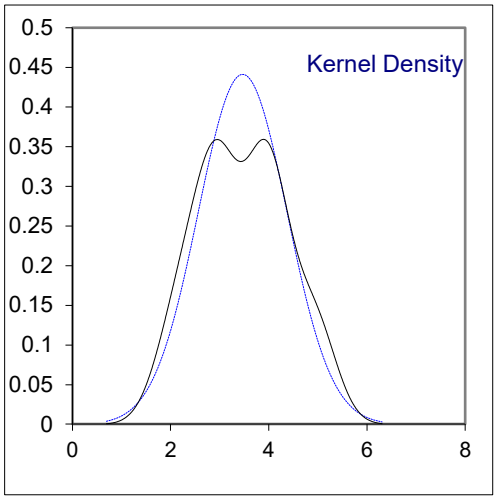
lab	method	value	mark	z(targ)	remarks
169		-----		-----	
171	IMPCA002	<0.25		-----	
174		-----		-----	
315	INH-158	<0.2		-----	
323	IMPCA002	<0.25		-----	
343		-----		-----	
345		-----		-----	
349		-----		-----	
396		-----		-----	
444		-----		-----	
551		-----		-----	
557		-----		-----	
657		-----		-----	
886		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016		-----		-----	
1069		-----		-----	
1429	ISO6227	<1		-----	
1530		-----		-----	
6198		-----		-----	
6201		-----		-----	
6438		-----		-----	
	n	4			
	mean (n)	<1			

Determination of Color Pt/Co on sample #23165;

lab	method	value	mark	z(targ)	remarks
169	D5386	4		0.21	
171	D1209	5		0.61	
174	D5386	4.0		0.21	
315	D1209	<5		-----	
323	D1209	<5		-----	
343	D1209	<5		-----	
345	D1209	4		0.21	
349	D5386	2.6		-0.35	
396	D5386	3		-0.19	
444	D5386	2.3		-0.47	
551	D1209	2		-0.59	
557		-----		-----	
657	D1209	3		-0.19	
886	D1209	3		-0.19	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016	D1209	4		0.21	
1069	D1209	3		-0.19	
1429	D1209	<5		-----	
1530		-----		-----	
6198	D5386	4.85		0.55	
6201	D5386	3.8		0.13	
6438		-----		-----	

normality	OK
n	14
outliers	0
mean (n)	3.47
st.dev. (n)	0.905
R(calc.)	2.53
st.dev.(D1209:05R19)	2.5
R(D1209:05R19)	7

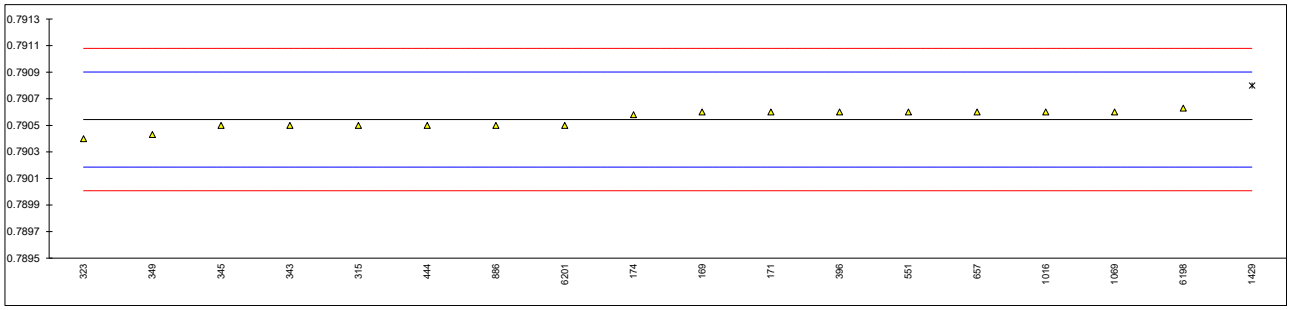


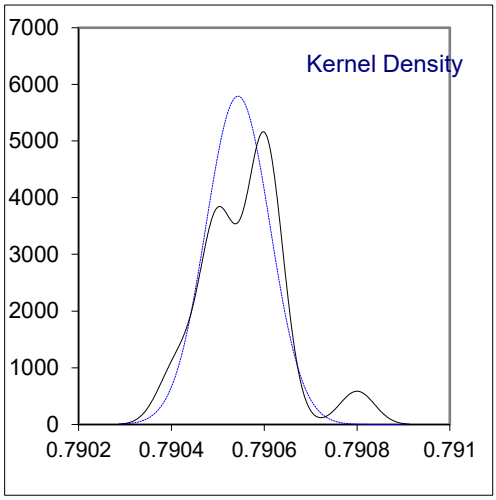


Determination of Density at 20 °C on sample #23165; results in kg/L

lab	method	value	mark	z(targ)	remarks
169	D4052	0.7906		0.32	
171	D4052	0.7906		0.32	
174	D4052	0.79058		0.20	
315	D4052	0.7905		-0.24	
323	D4052	0.7904		-0.80	
343	D4052	0.7905		-0.24	
345	D4052	0.7905		-0.24	
349	D4052	0.79043		-0.64	
396	D4052	0.7906		0.32	
444	D4052	0.7905		-0.24	
551	D4052	0.7906		0.32	
557		-----		-----	
657	D4052	0.7906		0.32	
886	D4052	0.7905		-0.24	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016	ISO12185	0.7906		0.32	
1069	D4052	0.7906		0.32	
1429	D4052	0.7908	G(0.05)	1.44	
1530		-----		-----	
6198	D4052	0.7906		0.48	
6201	D4052	0.7905		-0.24	
6438		-----		-----	

normality	OK
n	17
outliers	1
mean (n)	0.79054
st.dev. (n)	0.000069
R(calc.)	0.00019
st.dev.(ISO12185:96)	0.000179
R(ISO12185:96)	0.0005

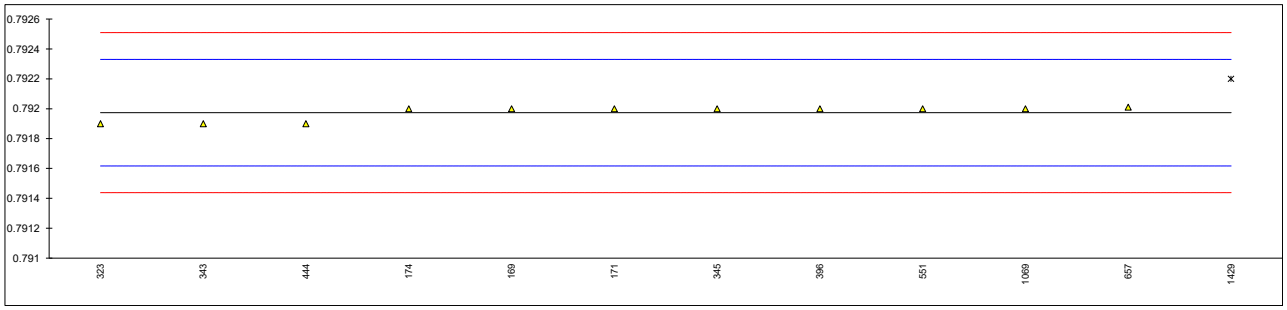


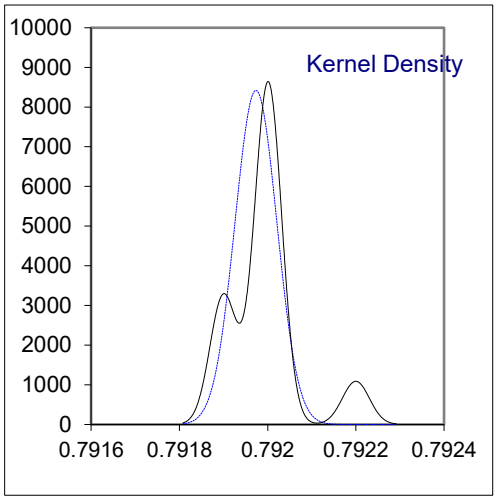


Determination of Specific Gravity 20/20 °C on sample #23165;

lab	method	value	mark	z(targ)	remarks
169	D4052	0.7920		0.15	
171	D4052	0.7920		0.15	
174	D4052	0.7920		0.15	
315		-----		-----	
323	D4052	0.7919		-0.41	
343	D4052	0.7919		-0.41	
345	D4052	0.7920		0.15	
349		-----		-----	
396	D4052	0.7920		0.15	
444	D4052	0.7919		-0.41	
551	D4052	0.7920		0.15	
557		-----		-----	
657	D4052	0.79201		0.20	
886		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016		-----		-----	
1069	D4052	0.7920		0.15	
1429	D4052	0.7922	G(0.05)	1.27	
1530		-----		-----	
6198		-----		-----	
6201		-----		-----	
6438		-----		-----	

normality	OK
n	11
outliers	1
mean (n)	0.79197
st.dev. (n)	0.000047
R(calc.)	0.00013
st.dev.(ISO12185:96)	0.000179
R(ISO12185:96)	0.0005

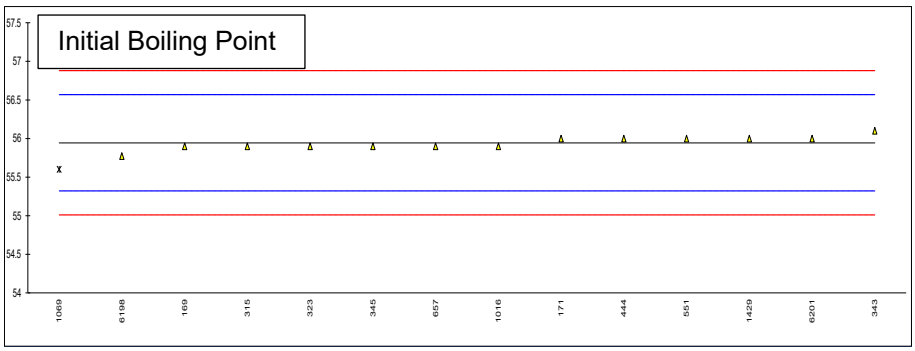


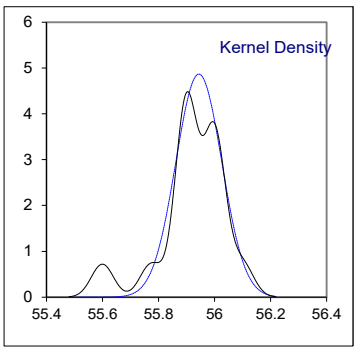


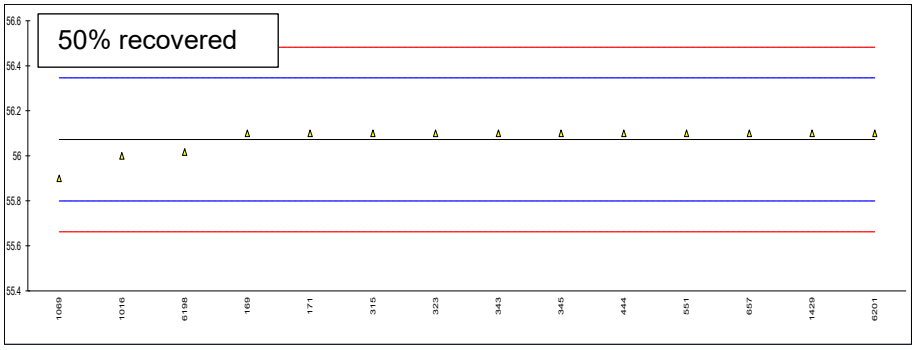
Determination of Initial Boiling point, 50% recovered and Dry Point on sample #23165; results in °C

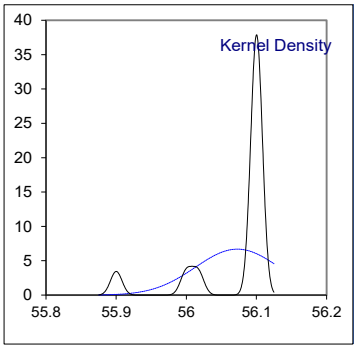
lab	method	IBP	mark	z(targ)	50% rec.	mark	z(targ)	DP	mark	z(targ)	range
169	D1078-automated	55.9		-0.14	56.1		0.20	56.3		-0.01	0.4
171	D1078-automated	56.0		0.18	56.1		0.20	56.2		-0.47	0.2
174		-----		-----	-----		-----	-----		-----	-----
315	D1078-automated	55.9		-0.14	56.1		0.20	56.3		-0.01	0.4
323	D1078-automated	55.9		-0.14	56.1		0.20	56.3		-0.01	0.4
343	D1078-automated	56.1		0.50	56.1		0.20	56.3		-0.01	0.2
345	D1078-automated	55.9		-0.14	56.1		0.20	56.3		-0.01	0.4
349		-----		-----	-----		-----	-----		-----	-----
396		-----		-----	-----		-----	-----		-----	-----
444	D1078-automated	56.0		0.18	56.1		0.20	56.3		-0.01	0.3
551	D1078-automated	56.0		0.18	56.1		0.20	56.3		-0.01	0.3
557		-----		-----	-----		-----	-----		-----	-----
657	D1078-automated	55.9		-0.14	56.1		0.20	56.2		-0.47	0.3
886		-----		-----	-----		-----	-----		-----	-----
913		-----		-----	-----		-----	-----		-----	-----
962		-----		-----	-----		-----	-----		-----	-----
963		-----		-----	-----		-----	-----		-----	-----
1016	D1078-automated	55.9		-0.14	56.0		-0.53	56.5		0.92	-----
1069	D1078-automated	55.6	G(5)	-1.10	55.9		-1.26	56.3		-0.01	0.7
1429	D1078-automated	56.0		0.18	56.1		0.20	56.3		-0.01	0.3
1530		-----		-----	-----		-----	-----		-----	-----
6198	D1078	55.774		-0.55	56.0165		-0.41	56.326		0.11	0.552
6201	D1078-manual	56.0		0.18	56.1		0.20	56.3		-0.01	0.3
6438		-----		-----	-----		-----	-----		-----	-----

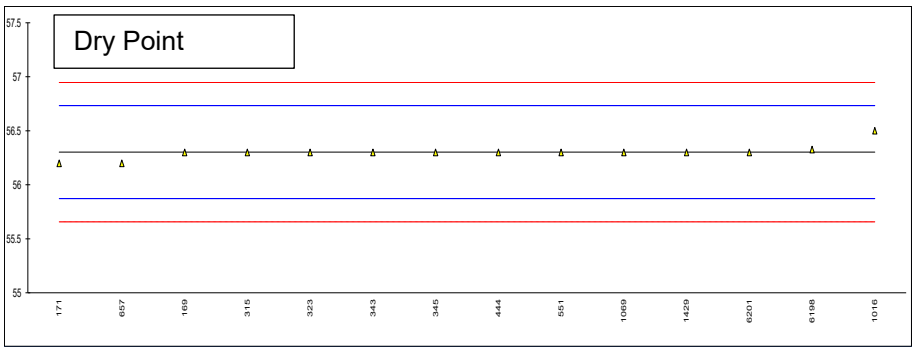
	normality	OK	not OK	not OK
	n	13	14	14
	outliers	1	0	0
	mean (n)	55.94	56.07	56.30
	st.dev. (n)	0.082	0.060	0.068
	R(calc.)	0.23	0.17	0.19
	st.dev.(D1078-A:11R19)	0.312	0.137	0.215
	R(D1078-A:11R19)	0.87	0.38	0.60
compare				
	R(D1078-M:11R19)	0.60	0.36	0.73

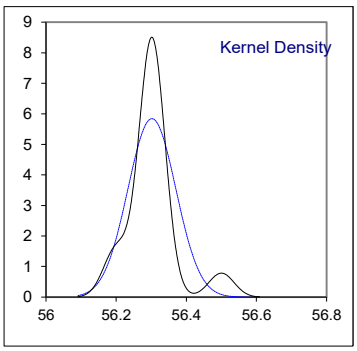

Initial Boiling Point
57.5
57
56.5
56
55.5
55
54.5
54
1069
6198
169
315
323
345
657
1016
171
444
551
1429
6201
343


Kernel Density
6
5
4
3
2
1
0
55.4
55.6
55.8
56
56.2
56.4


50% recovered
56.6
56.4
56.2
56
55.8
55.6
55.4
1069
1016
6198
169
171
315
323
343
345
444
551
657
1429
6201


Kernel Density
40
35
30
25
20
15
10
5
0
55.8
55.9
56
56.1
56.2


Dry Point
57.5
57
56.5
56
55.5
55
171
657
169
315
323
343
345
444
551
1069
1429
6201
6198
1016


Kernel Density
9
8
7
6
5
4
3
2
1
0
56
56.2
56.4
56.6
56.8

Determination of Water miscibility (Hydrocarbons) on sample #23165;

lab	method	value	mark	z(targ)	remarks
169	D1722	passes test		-----	
171	D1722	Pass		-----	
174	D1722	Pass		-----	
315	D1722	pass		-----	
323	D1722	PASS		-----	
343		-----		-----	
345	D1722	passes test		-----	
349		-----		-----	
396	D1722	Pass		-----	
444	D1722	Pass		-----	
551	D1722	Pass		-----	
557		-----		-----	
657	D1722	Pass		-----	
886		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016	D1722	Pass		-----	
1069	D1722	passes test		-----	
1429		-----		-----	
1530		-----		-----	
6198	D1722	Pass		-----	
6201	D1722	PASS		-----	
6438		-----		-----	
	n	14			
	mean (n)	Pass			

Determination of Nonvolatile matter on sample #23165; results in mg/100 mL

lab	method	value	mark	z(targ)	remarks
169	D1353	0		-----	
171	D1353	0.5		-----	
174		-----		-----	
315	D1353	<1		-----	
323	D1353	<1.0		-----	
343	D1353	<0.1		-----	
345	D1353	<0.1		-----	
349		-----		-----	
396		-----		-----	
444	D1353	<1		-----	
551		-----		-----	
557		-----		-----	
657	D1353	0.2		-----	
886		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016	D1353	0.3		-----	
1069	D1353	0		-----	
1429		-----		-----	
1530		-----		-----	
6198		-----		-----	
6201	D1353	4	C	-----	First reported 10.0, possibly a false positive test result?
6438		-----		-----	
	n	10			
	mean (n)	<1			

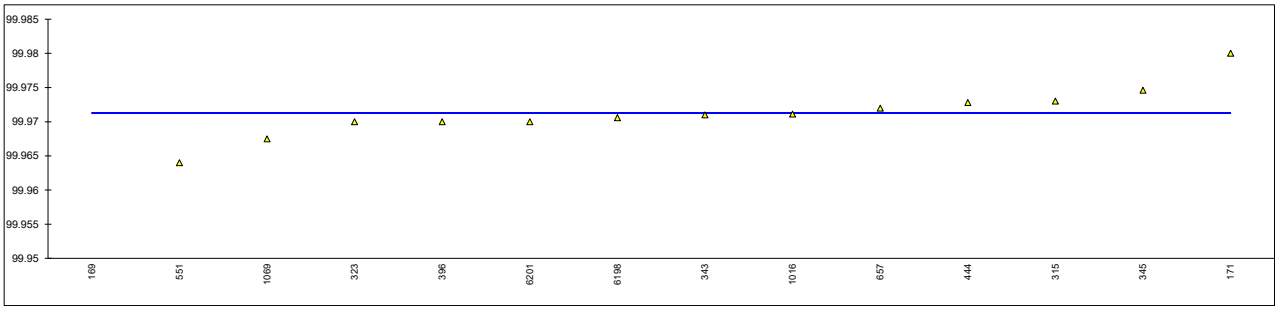
Determination of Permanganate Time Test at 25 °C on sample #23165; results in minutes

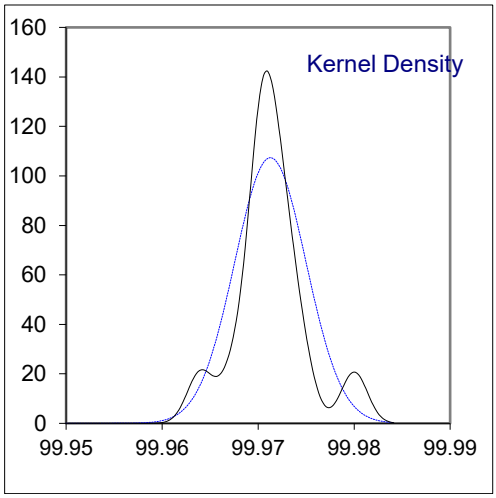
lab	method	value	mark	z(targ)	remarks
169	D1363	>30		-----	
171	D1363	100		-----	
174	D1363	77		-----	
315	D1363	90		-----	
323	D1363	>30		-----	
343	D1363	>30		-----	
345		-----		-----	
349		-----		-----	
396		-----		-----	
444	D1363	335		-----	
551	D1363	63		-----	
557		-----		-----	
657	D1363	70		-----	
886		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016	D1363	90		-----	
1069	D1363	103		-----	
1429		-----		-----	
1530		-----		-----	
6198		-----		-----	
6201	D1363	95		-----	
6438		-----		-----	
	n	12			
	mean (n)	>30			

Determination of Purity by GC on dry basis on sample #23165, results in %M/M

lab	method	value	mark	z(targ)	remarks
169		99.91	C,G(0.01)	-----	First reported 99.73
171	INH-001	99.98		-----	
174		-----		-----	
315	INH-394	99.973		-----	
323	INH-020	99.97		-----	
343	INH-4011	99.9710	C	-----	First reported 99.7591
345	INH-023	99.9746		-----	
349		-----		-----	
396	INH-0557	99.97		-----	
444	INH-020	99.9728		-----	
551	INH-1368	99.964		-----	
557		-----		-----	
657	INH-009	99.972		-----	
886		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016	DIN55687	99.97111		-----	
1069	In house	99.9675		-----	
1429		-----		-----	
1530		-----		-----	
6198	GB/T 6026	99.9706		-----	
6201		99.97		-----	
6438		-----		-----	

	normality	not OK
	n	13
	outliers	1
	mean (n)	99.971
	st.dev. (n)	0.0037
	R(calc.)	0.010
	st.dev.(lit)	unknown
	R(lit)	unknown
compare		
	R(iis21C11)	0.025

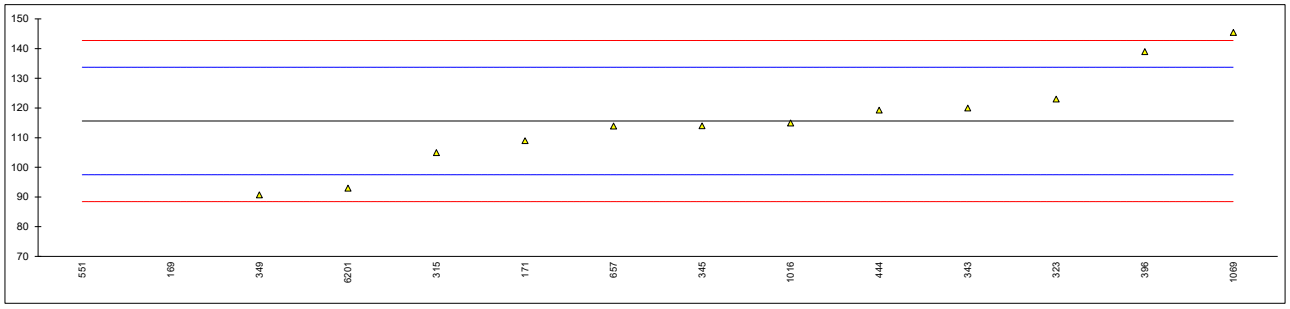


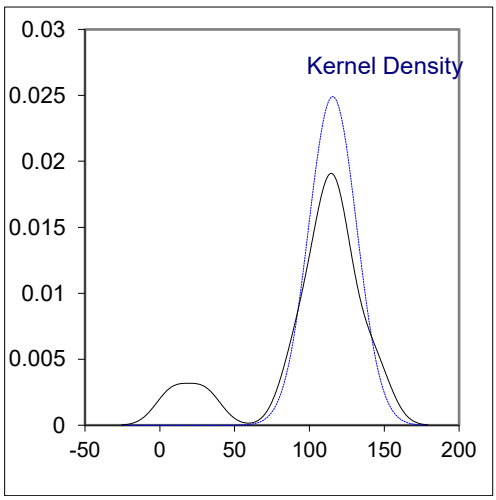


Determination of Diacetone alcohol on sample #23165, results in mg/kg

lab	method	value	mark	z(targ)	remarks
169		30	C,DG(0.01)	-9.46	First reported 0
171	INH-001	109		-0.73	
174		-----		-----	
315	INH-394	105		-1.17	
323	INH-020	123		0.82	
343	INH-4011	120		0.49	
345	INH-023	114		-0.18	
349	INH-CM034	90.7		-2.75	
396	INH-0557	139		2.58	
444	INH-020	119.3		0.41	
551	INH-1368	8.3	DG(0.01)	-11.86	
557		-----		-----	
657	INH-009	113.9		-0.19	
886		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016	DIN55687	114.931		-0.08	
1069	In house	145.5		3.30	
1429		-----		-----	
1530		-----		-----	
6198		-----		-----	
6201		93		-2.50	
6438		-----		-----	

normality	OK
n	12
outliers	2
mean (n)	115.611
st.dev. (n)	16.0169
R(calc.)	44.847
st.dev.(Horwitz)	9.0491
R(Horwitz)	25.338

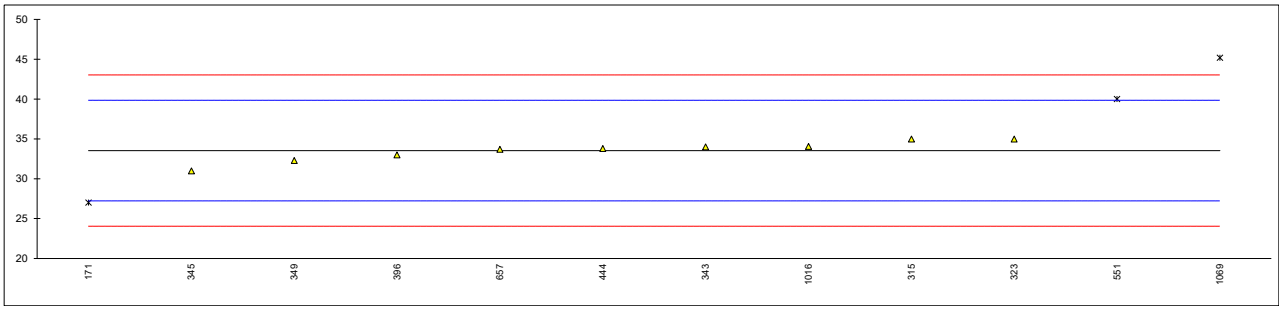


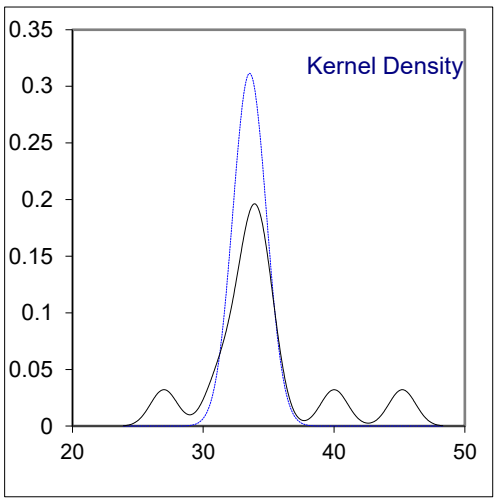


Determination of Mesityloxide on sample #23165, results in mg/kg

lab	method	value	mark	z(targ)	remarks
169		-----		-----	
171	INH-001	27	G(0.05)	-2.07	
174		-----		-----	
315	INH-394	35		0.46	
323	INH-020	35		0.46	
343	INH-4011	34		0.14	
345	INH-023	31		-0.80	
349	INH-CM034	32.3		-0.39	
396	INH-0557	33		-0.17	
444	INH-020	33.8		0.08	
551	INH-1368	40	DG(0.05)	2.04	
557		-----		-----	
657	INH-009	33.7		0.05	
886		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016	DIN55687	34.078		0.17	
1069	In house	45.2	DG(0.05)	3.69	
1429		-----		-----	
1530		-----		-----	
6198		-----		-----	
6201		-----		-----	
6438		-----		-----	

normality	OK
n	9
outliers	3
mean (n)	33.54
st.dev. (n)	1.282
R(calc.)	3.59
st.dev.(Horwitz)	3.163
R(Horwitz)	8.86

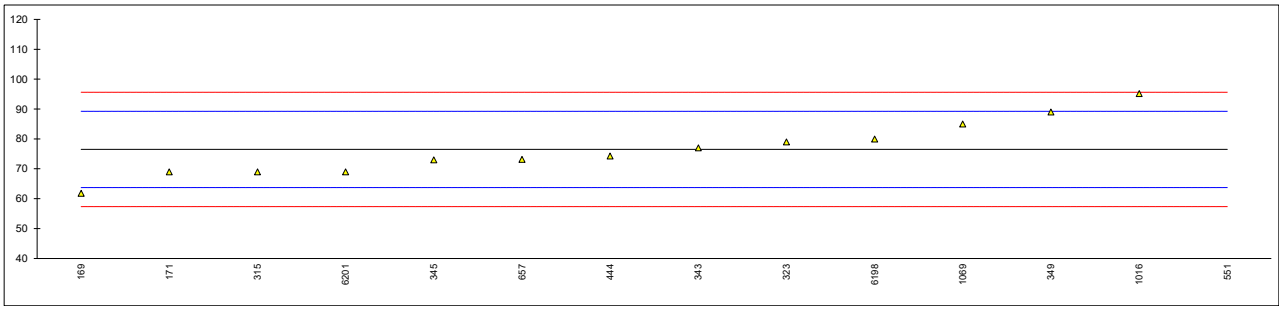


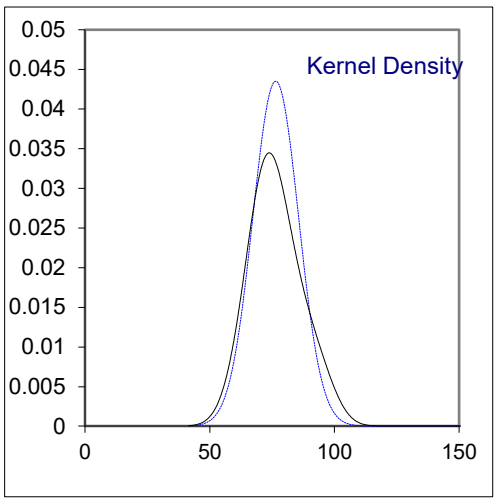


Determination of Methanol on sample #23165, results in mg/kg

lab	method	value	mark	z(targ)	remarks
169		61.8	C	-2.31	First reported 0.00618 mg/kg
171	INH-001	69		-1.18	
174		-----		-----	
315	INH-394	69		-1.18	
323	INH-020	79		0.39	
343	INH-4011	77		0.08	
345	INH-023	73		-0.55	
349	INH-CM034	89	C	1.96	First reported 101.5
396		-----		-----	
444	INH-020	74.3		-0.35	
551	INH-1368	183	G(0.01)	16.71	
557		-----		-----	
657	INH-009	73.2		-0.52	
886		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016	DIN55687	95.191		2.93	
1069	In house	85.0		1.33	
1429		-----		-----	
1530		-----		-----	
6198	GB/T 6026	80		0.55	
6201		69		-1.18	
6438		-----		-----	

normality	OK
n	13
outliers	1
mean (n)	76.50
st.dev. (n)	9.172
R(calc.)	25.68
st.dev.(Horwitz)	6.372
R(Horwitz)	17.84

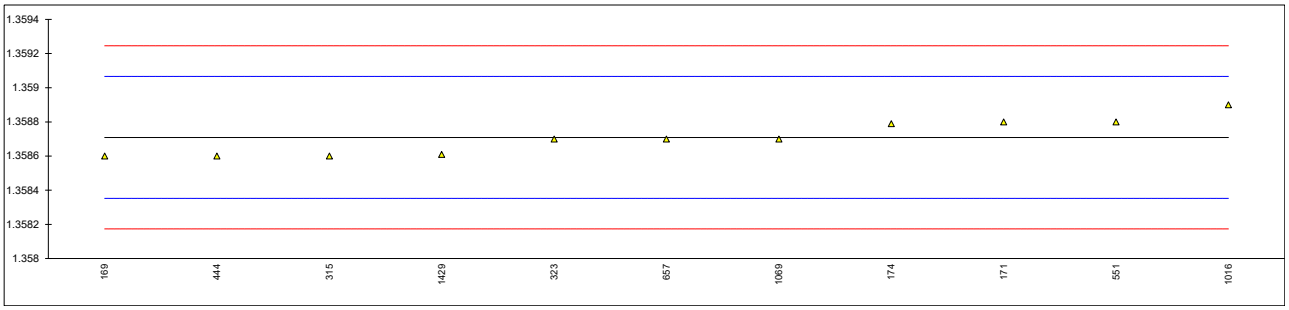


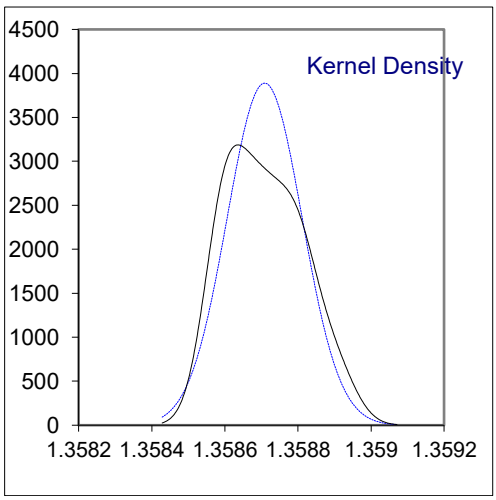


Determination of Refractive Index at 20 °C on sample #23165;

lab	method	value	mark	z(targ)	remarks
169	D1218	1.3586		-0.61	
171	D1218	1.3588	C	0.51	First reported 1.3606
174	D1218	1.35879		0.45	
315	D1218	1.3586		-0.61	
323	D1218	1.3587		-0.05	
343		-----		-----	
345		-----		-----	
349		-----		-----	
396		-----		-----	
444	D1218	1.3586		-0.61	
551	D1218	1.3588		0.51	
557		-----		-----	
657	D1218	1.35870		-0.05	
886		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016		1.3589		1.07	
1069	D1218	1.35870		-0.05	
1429	D1218	1.35861		-0.55	
1530		-----		-----	
6198		-----		-----	
6201		-----		-----	
6438		-----		-----	

normality	OK
n	11
outliers	0
mean (n)	1.35871
st.dev. (n)	0.000103
R(calc.)	0.00029
st.dev.(D1218:21)	0.000179
R(D1218:21)	0.0005

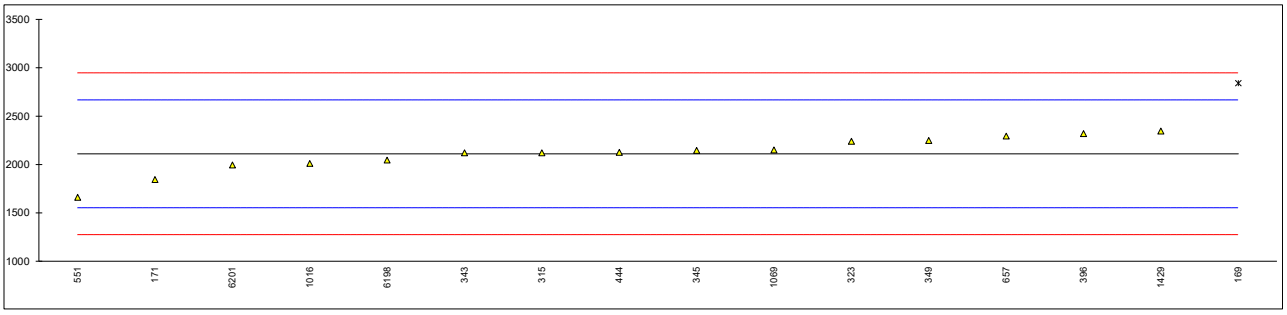


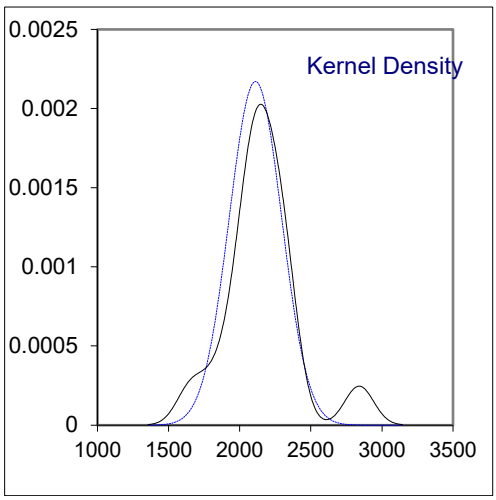


Determination of Water on sample #23165; results in mg/kg

lab	method	value	mark	z(targ)	remarks
169	E203	2840	C,G(0.05)	2.62	First reported 0.284 mg/kg
171	E203	1845	C	-0.95	First reported 0.184 mg/kg
174		-----		-----	
315	E203	2120		0.03	
323	E203	2239	C	0.46	First reported 0.224 mg/kg
343	E203	2120		0.03	
345	D1364	2145		0.12	
349	D1364	2248		0.49	
396	D1364	2320		0.75	
444	E203	2125		0.05	
551	E203	1660		-1.62	
557		-----		-----	
657	E203	2293	C	0.65	First reported 3133
886		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1016	D1364	2010		-0.36	
1069	D1364	2150		0.14	
1429	E203	2346		0.84	
1530		-----		-----	
6198	D1364	2044.5		-0.24	
6201	D1364	1994	C	-0.42	First reported 0.1994 mg/kg
6438		-----		-----	

normality	suspect
n	15
outliers	1
mean (n)	2110.63
st.dev. (n)	183.748
R(calc.)	514.49
st.dev.(E203:23)	278.571
R(E203:23)	780





APPENDIX 2

Number of participants per country

1 lab in BELGIUM
2 labs in BRAZIL
1 lab in CHINA, People's Republic
1 lab in FINLAND
1 lab in GERMANY
1 lab in INDIA
1 lab in ITALY
3 labs in NETHERLANDS
3 labs in SAUDI ARABIA
1 lab in SINGAPORE
3 labs in SPAIN
1 lab in TAIWAN
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)/D(1)	= outlier in Dixon's outlier test
D(0.05)/D(5)	= straggler in Dixon's outlier test
G(0.01)/G(1)	= outlier in Grubbs' outlier test
G(0.05)/G(5)	= straggler in Grubbs' outlier test
DG(0.01)/DG(1)	= outlier in Double Grubbs' outlier test
DG(0.05)/DG(5)	= straggler in Double Grubbs' outlier test
R(0.01)/R(1)	= outlier in Rosner's outlier test
R(0.05)/R(5)	= 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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