Results of Proficiency Test
n-Butyl Acetate
March 2019

Organised by: Institute for Interlaboratory Studies
Spijkenisse, the Netherlands

Author: A. Lewinska, MSc.
Correctors: ing. A.S. Noordman-de Neef & ing. R.J. Starink
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CONTENTS

1 INTRODUCTION

Since 2015, the Institute for Interlaboratory Studies (iis) organizes proficiency tests for n-Butyl Acetate every two year. During the annual proficiency testing program of 2018/2019, it was decided to continue the proficiency tests for the analysis of n-Butyl Acetate.
In this interlaboratory study in total 14 laboratories in 11 different countries did register for participation. See appendix 2 for the number of participants per country.
In this report, the results of the 2019 proficiency test for n-Butyl Acetate 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 organiser of this proficiency test (PT). Sample analyses for fit-for-use and homogeneity testing were subcontracted to an ISO/IEC17025 accredited laboratory.
It was decided to send one sample of 0.5L of n-Butyl Acetate, labelled #19040.
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 organisation 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 SAMPLE

The necessary bulk material of n-Butyl Acetate was obtained from a local chemical supplier. After homogenisation, 40 amber glass bottles of 0.5L were filled and labelled #19040.
The homogeneity of the subsamples was checked by determination of Density at 20°C in accordance with ASTM D4052 on 4 stratified randomly selected samples.

	Density at 20°C in kg/L
sample #19040-1	0.88124
sample #19040-2	0.88124
sample #19040-3	0.88124
sample #19040-4	0.88123

Table 1: homogeneity test results of subsamples #19040

From the above test results the repeatability was calculated and compared with 0.3 times the corresponding reproducibility of the reference test method in agreement with the procedure of ISO 13528, Annex B2 in the next table.

	Density at 20°C in kg/L
r (observed)	0.00001
Reference test method	ISO12185:96
0.3*R (reference test method)	0.00015

Table 2: evaluation of the repeatabilities of subsamples #19040

The calculated repeatability was in agreement with 0.3 times the corresponding reproducibility of the reference test method. Therefore, homogeneity of the subsamples #19040 was assumed.

To each of the participating laboratories one 0.5L bottle of n-Butyl Acetate labelled #19040 was sent on March 13, 2019. An SDS was added to the sample package.

2.5 STABILITY OF THE SAMPLE

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

2.6 ANALYSES

The participants were asked to determine on sample #19040: Acidity as Acetic Acid, Color Pt/Co, Density at 20°C, Specific Gravity 20/20°C, Distillation (IBP, 50% recovery, Dry Point and Distillation Range), Nonvolatile matter, Purity of n-Butyl Acetate, n-Butanol 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 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 reanalyses). Additional or corrected test results are used for data analysis and the original test results are placed under 'Remarks' in the test result tables in appendix 1. Test results that came in after the deadline were not taken into account in this screening for suspect data and thus these participants were not requested for checks.

3.1 STATISTICS

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

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

According to ISO5725 the original test results per determination were submitted to Dixon’s and/or Grubbs' and/or Rosner’s outlier tests. Outliers are marked by D(0.01) for the Dixon’s test, by G(0.01) or DG(0.01) for the Grubbs’ test and by R(0.01) for the Rosner’s test. Stragglers are marked by D(0.05) for the Dixon’s test, by G(0.05) or DG(0.05) for the Grubbs’ test and by R(0.05) for the Rosner’s test. Both outliers and stragglers were not included in the calculations of averages and standard deviations.

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

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

3.2 GRAPHICS

In order to visualize the data against the reproducibilities from literature, Gauss plots were made, using the sorted data for one determination (see appendix 1). On the Y-axis the reported test results are plotted. The corresponding laboratory numbers are on the X-axis.

The straight horizontal line presents the consensus value (a trimmed mean). The four striped lines, parallel to the consensus value line, are the +3s, +2s, -2s and -3s target reproducibility limits of the selected reference test method. Outliers and other data, which were excluded from the calculations, are represented as a cross. Accepted data are represented as a triangle.

Furthermore, Kernel Density Graphs were made. The Kernel Density Graph is a method for producing a smooth density approximation to a set of data that avoids some problems associated with histograms. Also, a normal Gauss curve was projected over the Kernel Density Graph for reference.

3.3 Z-SCORES

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

This target standard deviation was calculated from the literature reproducibility by division with 2.8. In case no literature reproducibility was available, other target values were used. In some cases, a reproducibility based on former iis proficiency tests could be used.

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

The z-scores were calculated according to:

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

The $z_{(target)}$ scores are listed in the result tables of 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 interlaboratory study, no major problems were encountered with dispatch of the samples. All reporting participants reported before the dead line. One participant did not report any test results.
In total 13 participants reported 112 numerical results. Observed was 1 outlying result, which is 0.9% of the total of numerical test results. In proficiency studies, outlier percentages of 3% - 7.5% are quite normal.

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

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 methods are also in the tables together with the original data. The abbreviations, used in these tables, are listed in appendix 3.

In the iis PT reports, ASTM 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(2011)). In the results tables of appendix 1 only the method number and year of adoption or revision e.g. D1209:05 will be used.

Sample #19040

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.

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

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

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: The determination of the Initial Boiling Point (IBP), 50% recovery and the Dry Point (DP) was not problematic. No statistical outliers were observed. The calculated reproducibilities are in agreement with the requirements of ASTM D1078:11 automated and manual method.
The determination of the Distillation Range was problematic. No statistical outliers were observed. However, the calculated reproducibility is not in agreement with the requirements of ASTM D1078:11 automated and manual method.

Nonvolatile matter: Eight participants reported a test result and agreed on a value for nonvolatile matter less or equal than 1 mg/100mL except one.
No z-scores were calculated because of the low amount of non-volatile matter.

Purity: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D3545:06(2012).

n-Butanol: This determination may be problematic. No statistical outliers were observed. However, the calculated reproducibility is not in agreement with the estimated reproducibility using the Horwitz equation.

Water: This determination was problematic. One statistical outlier was observed. However, the calculated reproducibility after rejection of the statistical outlier is not in agreement with the requirements of ASTM E1064:16.

4.2 PERFORMANCE EVALUATION FOR THE GROUP OF LABORATORIES

A comparison has been made between the reproducibility as declared by the relevant reference test method and the reproducibility as found for the group of participating laboratories. The number of significant test results, the average results, the calculated reproducibility (2.8 * standard deviation) and the target reproducibility derived from literature reference test methods (in casu ASTM, EN test methods) or previous proficiency tests are presented in the next tables.

Parameter	unit	n	average	2.8 * sd	R (target)
Acidity as Acetic Acid	mg/kg	13	9.1	10.7	14
Color Pt/Co		11	4	3	7
Density at 20°C	kg/L	12	0.8812	0.0001	0.0005
Specific Gravity 20/20°C		12	0.8828	0.0001	0.0005
Initial Boiling Point	°C	6	125.2	1.0	2.0
50% recovery	°C	6	126.1	0.3	0.9
Dry Point	°C	6	126.2	0.4	1.4
Distillation Range	°C	6	1.1	1.0	0.8
Nonvolatile matter	mg/100mL	7	≤1	n.a.	n.a.
Purity	%M/M	11	99.774	0.079	0.2
n-Butanol	mg/kg	11	1539	313	228
Water	mg/kg	12	148.2	37.1	23.6

Table 3: reproducibilities of tests on sample #19040

Without further statistical calculations it can be concluded that for a number of tests there is a good compliance of the group of participants with the relevant standards.
The problematic tests have been discussed in paragraph 4.1.

4.3 COMPARISON OF THE PROFICIENCY TEST OF MARCH 2019 WITH PREVIOUS PTS.

	March 2019	April 2017	April 2015
Number of reporting labs	13	15	12
Number of results reported	112	246	180
Number of statistical outliers	1	11	3
Percentage outliers	0.9%	4.5%	1.7%

Table 4: comparison with previous proficiency test.

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

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

	March 2019	April 2017	April 2015
Acidity as Acetic Acid	+	-	++
Color Pt/Co	++	+/-	+
Density at 20°C	++	++	+
Specific Gravity 20/20°C	++	++	+
Initial Boiling Point	++	+	++
50% recovery	++	++	++
Dry Point	++	++	++
Distillation Range	-	+/-	+
Nonvolatile matter	n.e.	-	--
Purity	++	+/-	+
n-Butanol	-	-	-
Water	-	+	++

Table 5: comparison determinations against the reference test method

The following performance categories were used:

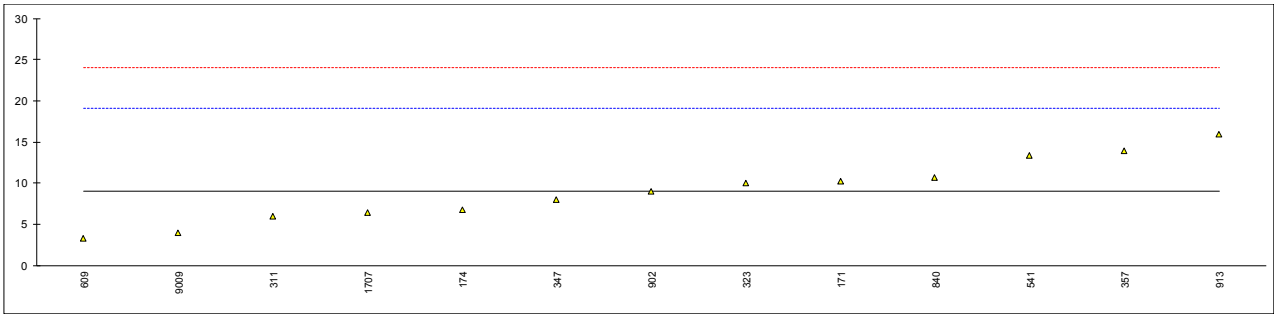
++: group performed much better than the reference test method
+ : group performed better than the s reference test method
+/-: group performance similar to the reference test method
- : group performed worse than the reference test method
-- : group performed much worse than the reference test method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

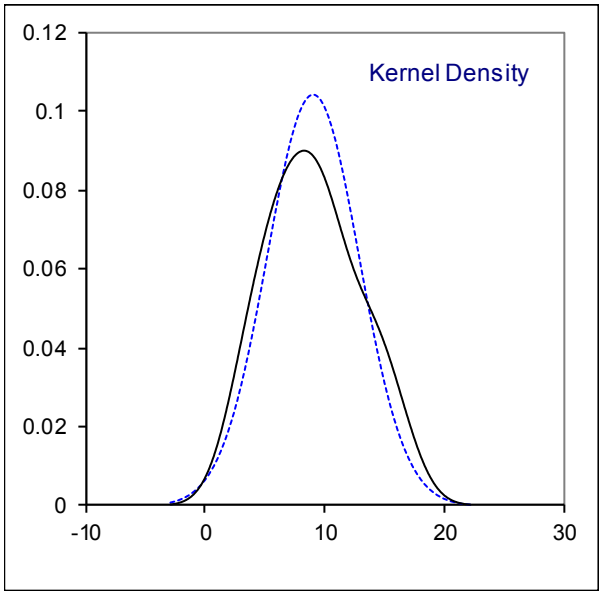
APPENDIX 1

Determination of Acidity as Acetic Acid on sample #19040; results in mg/kg

lab	method	value	mark	z(targ)	remarks
171	D1613	10.213		0.23	
174	D1613	6.8		-0.45	
311	D1613	6		-0.61	
323	D1613	10		0.19	
347	D1613	8		-0.21	
357	D1613	14		0.99	
541	D1613	13.4		0.87	
609	In house	3.36		-1.14	
840	D1613	10.7		0.33	
872		-----		-----	
902	D1613	9		-0.01	
913	D1613	16		1.39	
1707	D1613	6.5		-0.51	
9009	D1613	4		-1.01	

normality	OK
n	13
outliers	0
mean (n)	9.07
st.dev. (n)	3.836
R(calc.)	10.74
st.dev.(D1613:17)	5
R(D1613:17)	14

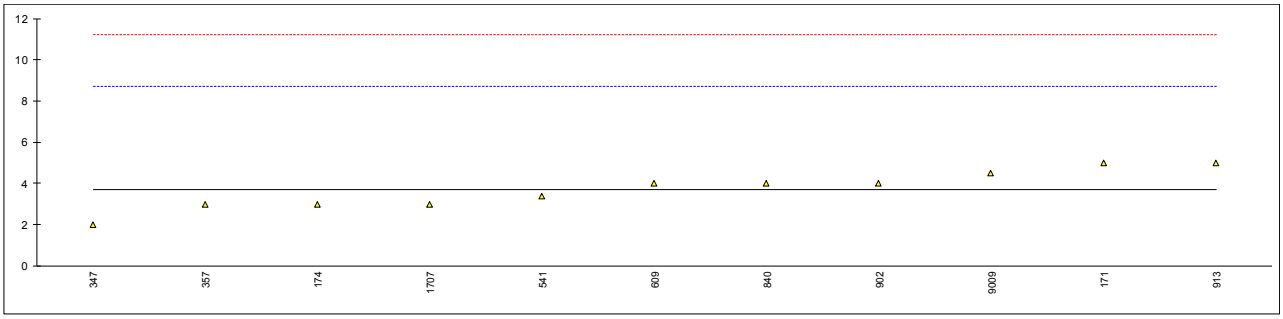


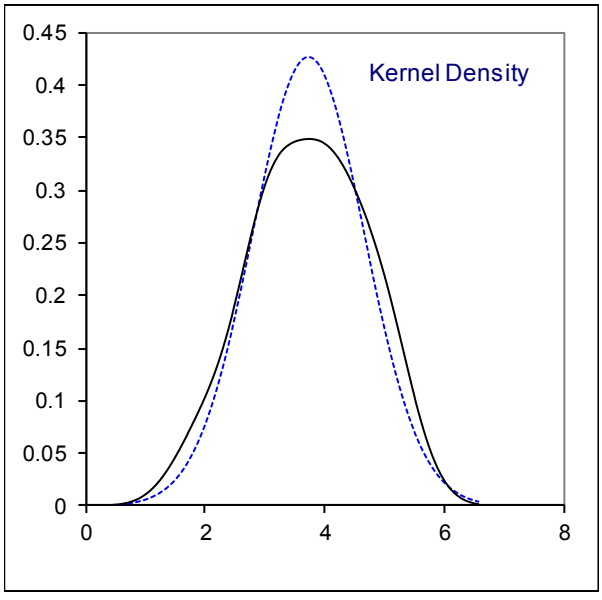


Determination of Color Pt/Co on sample #19040

lab	method	value	mark	z(targ)	remarks
171	D1209	5		0.51	
174	D5386	3.0		-0.29	
311	D1209	<5		-----	
323	D1209	<5		-----	
347	D5386	2		-0.69	
357	D5386	3		-0.29	
541	D5386	3.4		-0.13	
609	D5386	4		0.11	
840	D1209	4		0.11	
872		-----		-----	
902	D5386	4		0.11	
913	D5386	5		0.51	
1707	D5386	3.0		-0.29	
9009	D1209	4.5		0.31	

normality	OK
n	11
outliers	0
mean (n)	3.7
st.dev. (n)	0.93
R(calc.)	2.6
st.dev.(D1209:05)	2.50
R(D1209:05)	7

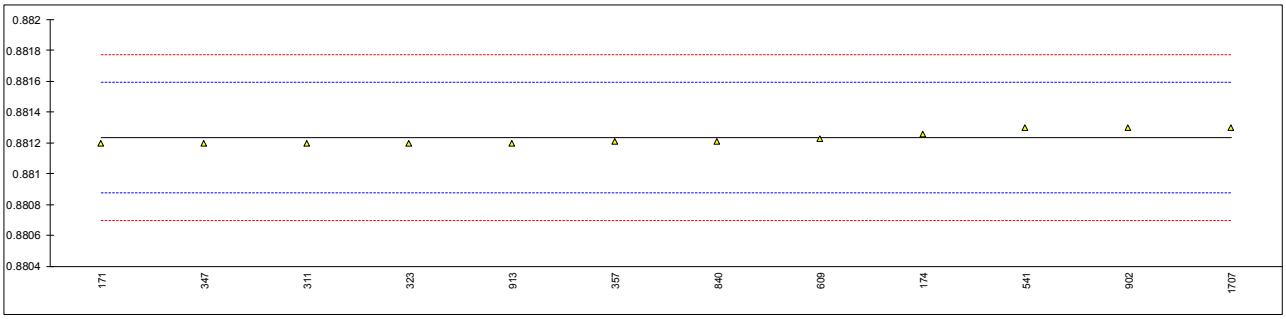


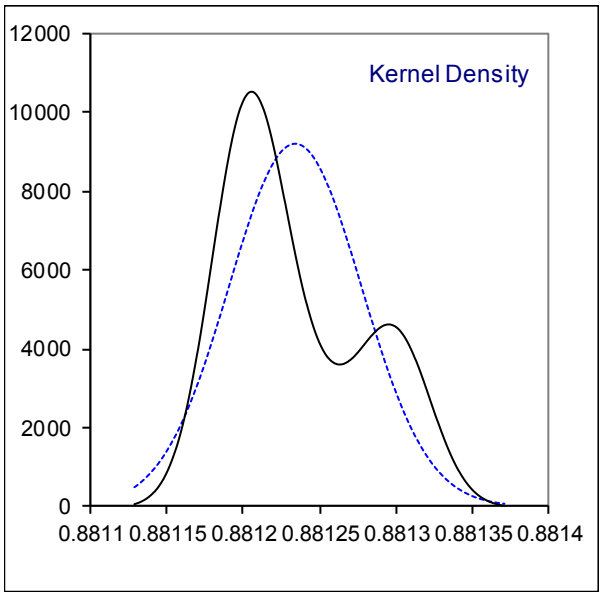


Determination of Density at 20°C on sample #19040; results in kg/L

lab	method	value	mark	z(targ)	remarks
171	D4052	0.8812		-0.19	
174	D4052	0.88126		0.14	
311	D4052	0.8812		-0.19	
323	D4052	0.8812		-0.19	
347	D4052	0.8812		-0.19	
357	D4052	0.88121		-0.14	
541	D4052	0.88130		0.37	
609	D4052	0.88123		-0.02	
840	D4052	0.88121		-0.14	
872		-----		-----	
902	ISO12185	0.8813		0.37	
913	D4052	0.8812		-0.19	
1707	D4052	0.8813		0.37	
9009		-----		-----	

normality	OK
n	12
outliers	0
mean (n)	0.88123
st.dev. (n)	0.000043
R(calc.)	0.00012
st.dev.(ISO12185:96)	0.000179
R(ISO12185:96)	0.0005
Compare	
R(D4052:18a)	0.0005

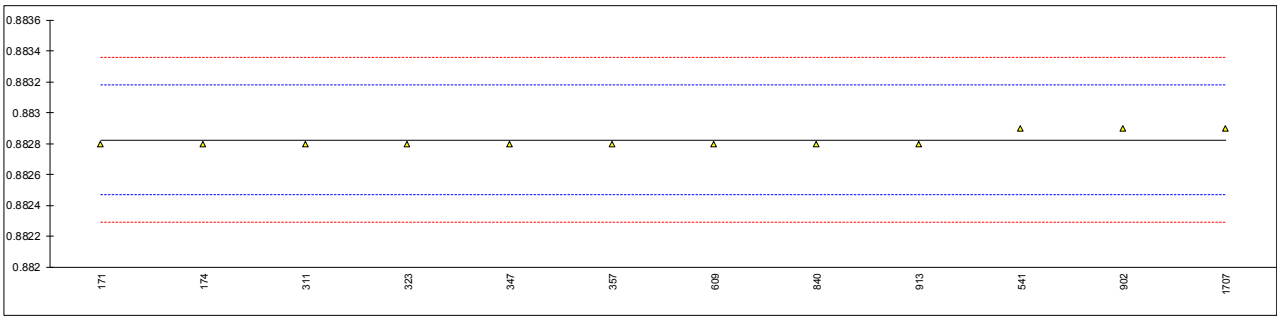


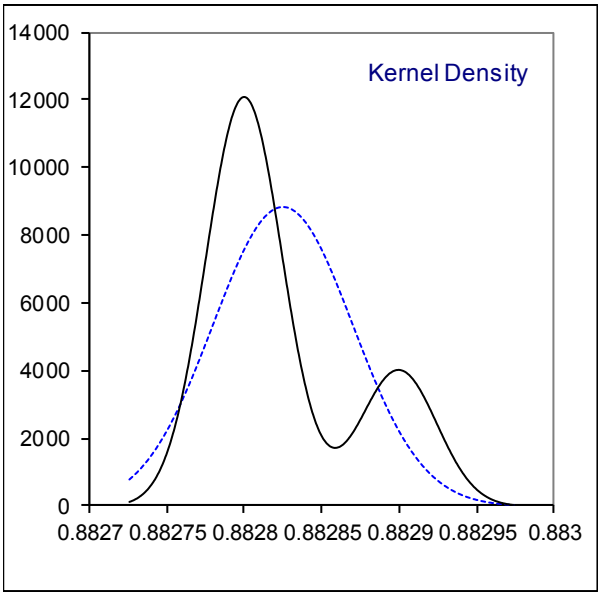


Determination of Specific Gravity 20/20°C on sample #19040

lab	method	value	mark	z(targ)	remarks
171	D4052	0.8828		-0.14	
174	D4052	0.8828		-0.14	
311	D4052	0.8828		-0.14	
323	D4052	0.8828		-0.14	
347	D4052	0.8828		-0.14	
357	D4052	0.8828		-0.14	
541	D4052	0.88290		0.42	
609	D4052	0.8828		-0.14	
840	D4052	0.88280		-0.14	
872		-----		-----	
902	ISO12185	0.8829		0.42	
913	D4052	0.8828		-0.14	
1707	D4052	0.8829		0.42	
9009		-----		-----	

normality	suspect
n	12
outliers	0
mean (n)	0.88283
st.dev. (n)	0.000045
R(calc.)	0.00013
st.dev.(ISO12185:96)	0.000179
R(ISO12185:96)	0.0005
Compare	
R(D4052:18a)	0.0005





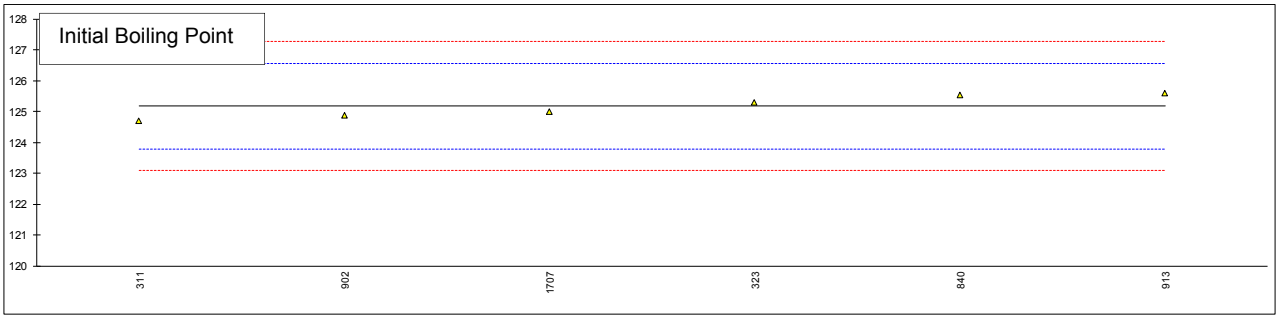
Determination of Distillation on sample #19040; results in °C

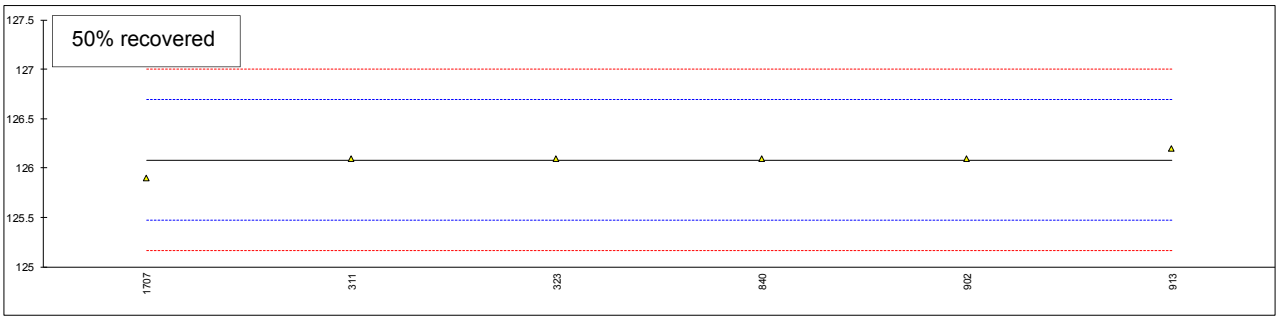
lab	method	IBP	mark	50% rec	mark	DP	mark	Distil. Range	mark
171		-----		-----		-----		-----	
174		-----		-----		-----		-----	
311		124.7		126.1		126.2		1.5	
323	D1078-automated	125.3		126.1		126.3		1.1	
347	D1078-automated	-----		-----		-----		-----	
357		-----		-----		-----		-----	
541		-----		-----		-----		-----	
609		-----		-----		-----		-----	
840	D1078-automated	125.54		126.10		126.15		0.61	
872		-----		-----		-----		-----	
902	D1078-automated	124.9		126.1		126.3		1.4	
913	D1078-manual	125.6		126.2		126.4		0.8	
1707	D1078-manual	125.0		125.9		126.0		1.0	
9009		-----		-----		-----		-----	
normality		unknown		unknown		unknown		unknown	
n		6		6		6		6	
outliers		0		0		0		0	
mean (n)		125.17		126.08		126.22		1.07	
st.dev. (n)		0.364		0.098		0.141		0.342	
R(calc.)		1.02		0.28		0.39		0.96	
st.dev.(D1078-A:11)		0.697		0.308		0.482		0.280	
R(D1078-A:11)		1.95		0.86		1.35		0.79	
Compare									
R(D1078-M:11)		1.34		0.82		1.64		0.71	

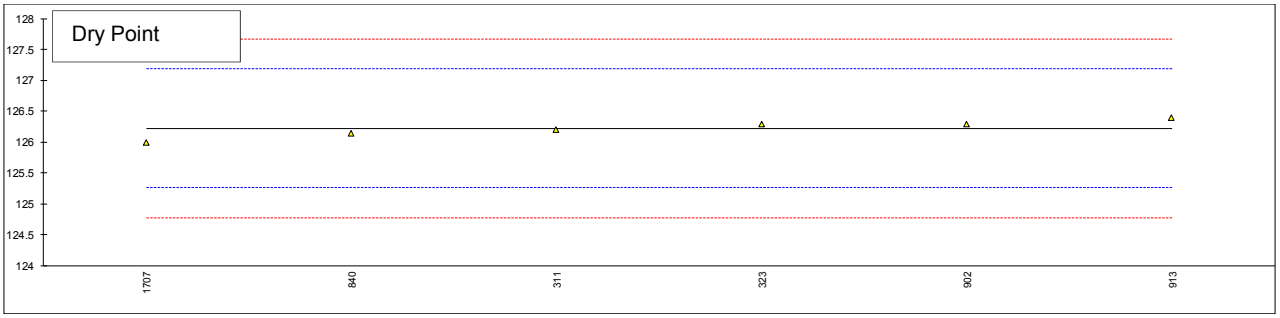
Theoretical mid boiling point = 126.1 °C

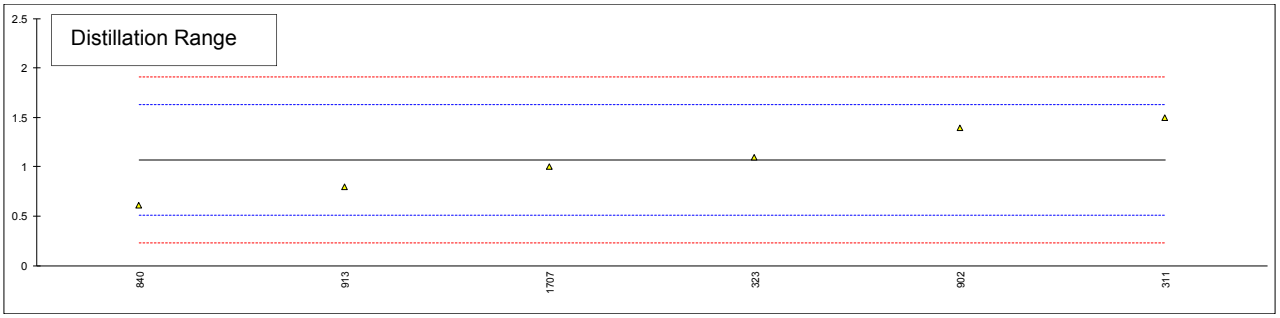
z-scores of Distillation on sample #19040

lab	method	IBP	50% rec	DP	Distil. Range
171		-----	-----	-----	-----
174		-----	-----	-----	-----
311		-0.68	0.05	-0.05	1.54
323	D1078-automated	0.18	0.05	0.16	0.11
347	D1078-automated	-----	-----	-----	-----
357		-----	-----	-----	-----
541		-----	-----	-----	-----
609		-----	-----	-----	-----
840	D1078-automated	0.53	0.05	-0.16	-1.63
872		-----	-----	-----	-----
902	D1078-automated	-0.39	0.05	0.16	1.18
913	D1078-manual	0.61	0.38	0.36	-0.96
1707	D1078-manual	-0.25	-0.60	-0.47	-0.24
9009		-----	-----	-----	-----


Initial Boiling Point
128
127
126
125
124
123
122
121
120
311
902
1707
323
840
913


50% recovered
127.5
127
126.5
126
125.5
125
1707
311
323
840
902
913


Dry Point
128
127.5
127
126.5
126
125.5
125
124.5
124
1707
840
311
323
902
913

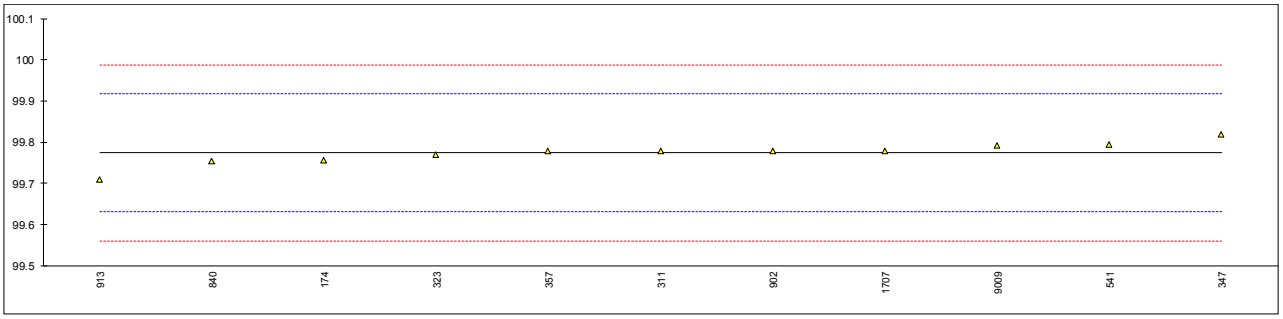

Distillation Range
2.5
2
1.5
1
0.5
0
840
913
1707
323
902
311

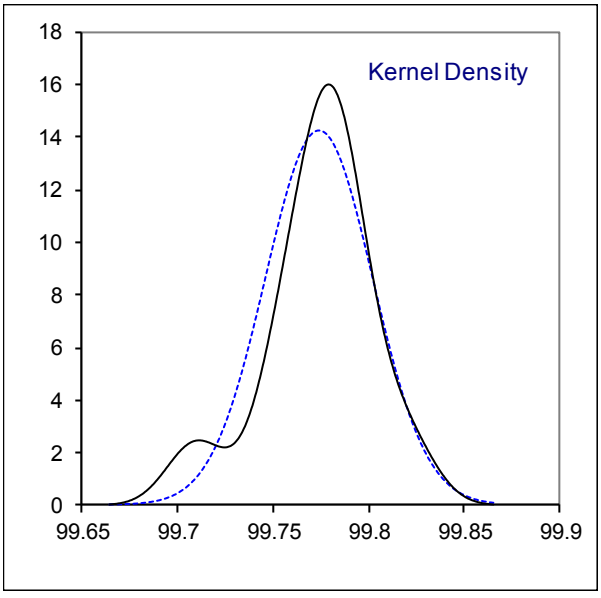
Determination of Nonvolatile matter on sample #19040; results in mg/100mL

lab	method	value	mark	z(targ)	remarks
171	D1353	0.100		-----	
174		-----		-----	
311	D1353	<1		-----	
323		-----		-----	
347		-----		-----	
357	D1353	1		-----	
541	D1353	<1	C	-----	first reported <0.001
609		-----		-----	
840	D1353	1.96		-----	possibly a false positive test result?
872		-----		-----	
902	D1353	1.0		-----	
913	D1353	<1		-----	
1707	D1353	0.8		-----	
9009		-----		-----	
	n	7			
	mean (n)	≤ 1			

Determination of Purity on sample #19040; results in %M/M

lab	method	value	mark	z(targ)	remarks
171		-----		-----	
174	INH-353	99.756		-0.26	
311	INH-172	99.78		0.08	
323	D3545	99.77		-0.06	
347	D3545	99.82		0.64	
357	D3545	99.779		0.07	
541	INH-1B	99.795		0.29	
609		-----		-----	
840	D3545	99.754		-0.28	
872		-----		-----	
902	INH-126	99.78		0.08	
913	D3545	99.71		-0.90	
1707	In house	99.78		0.08	
9009	In house	99.7925		0.26	
	normality	not OK			
	n	11			
	outliers	0			
	mean (n)	99.7742			
	st.dev. (n)	0.02805			
	R(calc.)	0.0785			
	st.dev.(D3545:06)	0.07143			
	R(D3545:06)	0.2			

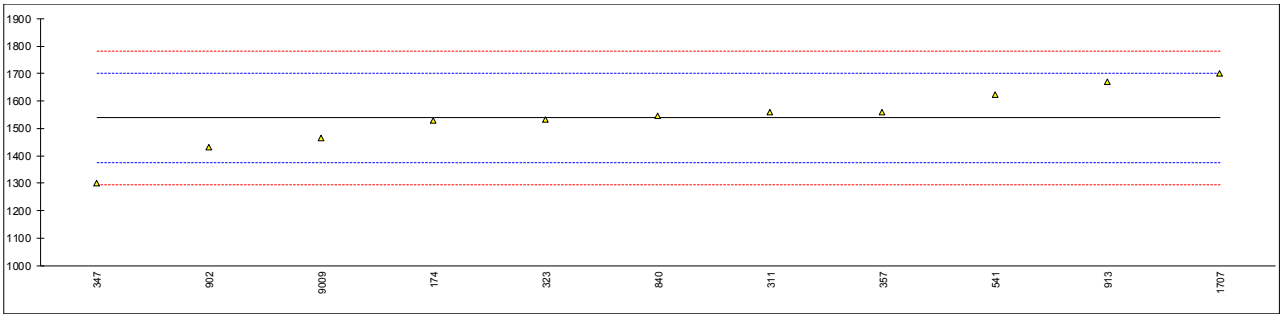


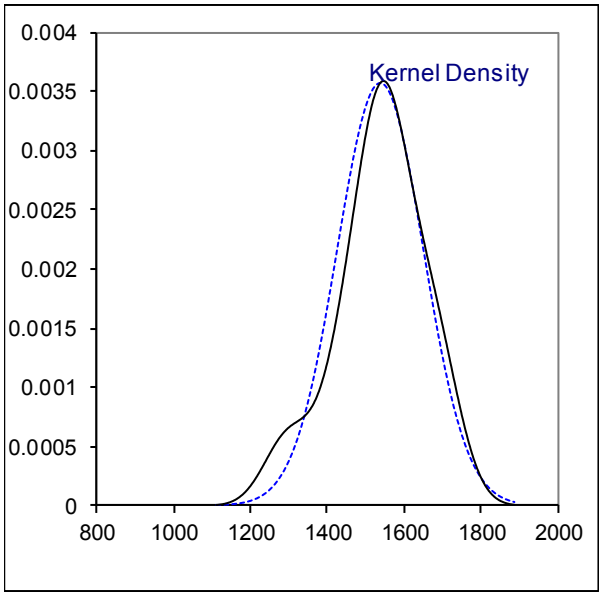


Determination of n-Butanol on sample #19040; results in mg/kg

lab	method	value	mark	z(targ)	remarks
171		-----		-----	
174	INH-353	1530		-0.11	
311	INH-172	1560		0.26	
323	D3545	1533		-0.07	
347	D3545	1300	C	-2.93	first reported 0.13 mg/kg
357	D3545	1560		0.26	
541	INH-1B	1623.8		1.04	
609		-----		-----	
840	D3545	1548		0.11	
872		-----		-----	
902	INH-126	1433		-1.30	
913	D3545	1671	C	1.62	first reported 0.1671 mg/kg
1707	In house	1700	C	1.98	first reported 0.17 mg/kg
9009	In house	1467		-0.88	

normality	suspect
n	11
outliers	0
mean (n)	1538.7
st.dev. (n)	111.87
R(calc.)	313.2
st.dev.(Horwitz)	81.58
R(Horwitz)	228.4

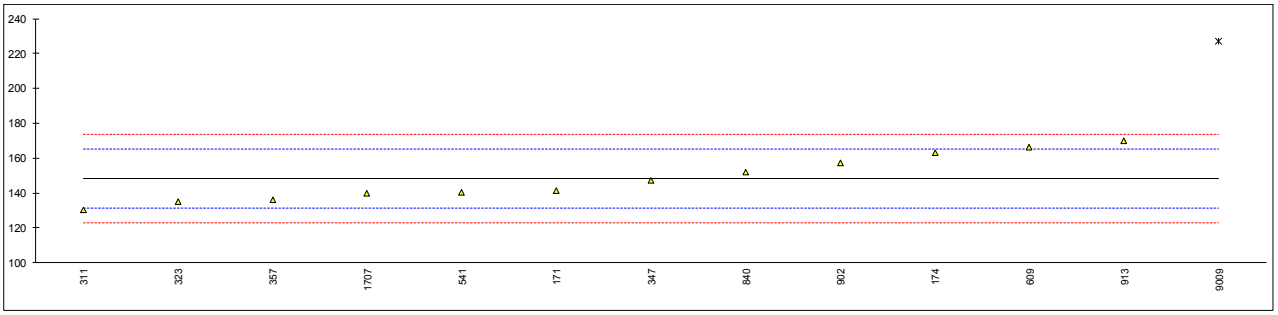


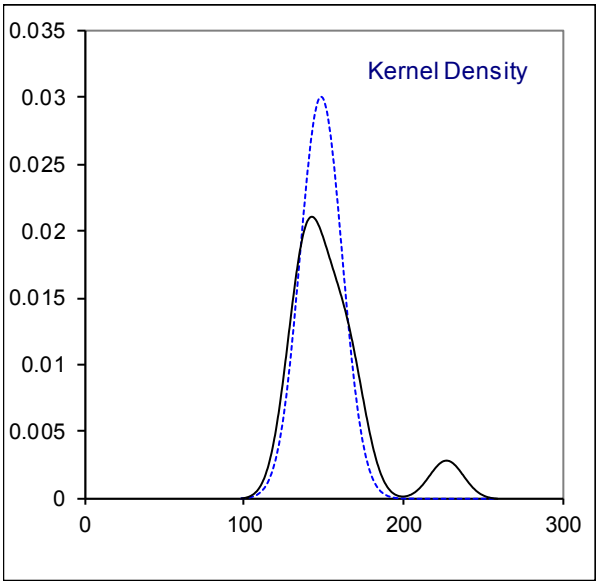


Determination of Water on sample #19040; results in mg/kg

lab	method	value	mark	z(targ)	remarks
171	E1064	141.41		-0.80	
174	E203	163		1.76	
311	E1064	130		-2.16	
323	E1064	135		-1.56	
347	E1064	147		-0.14	
357	E1064	136		-1.45	
541	E1064	140.5		-0.91	
609	E1064	166		2.12	
840	E1064	152.0		0.46	
872		-----		-----	
902	E1064	157		1.05	
913	E1064	170		2.60	
1707	E1064	140		-0.97	
9009	E1064	227	D(0.05)	9.37	

normality	OK
n	12
outliers	1
mean (n)	148.16
st.dev. (n)	13.251
R(calc.)	37.10
st.dev.(E1064:16)	8.413
R(E1064:16)	23.56





APPENDIX 2

Number of participants per country

1 lab in	ARGENTINA
1 lab in	BELGIUM
1 lab in	FINLAND
1 lab in	INDIA
2 labs in	MALAYSIA
1 lab in	NETHERLANDS
1 lab in	RUSSIAN FEDERATION
1 lab in	SPAIN
2 labs in	TURKEY
2 labs in	UNITED STATES OF AMERICA
1 lab in	VIETNAM

APPENDIX 3

Abbreviations:

C	= final 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)/R(1)	= outlier in Rosner's outlier test
R(0.05)/R(5)	= straggler in Rosner's outlier test
E	= possibly an error in calculations
W	= test result withdrawn on request of participant
ex	= test result excluded from statistical evaluation
n.a.	= not applicable
n.e.	= not evaluated
n.d.	= not detected
fr.	= first reported
SDS	= Safety Data Sheet

Literature:

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