Results of Proficiency Test
Benzene
March 2018

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1   INTRODUCTION

Since 1999, the Institute for Interlaboratory Studies (iis) organizes proficiency tests for the analysis of Benzene every year. During the annual proficiency testing program 2017/2018, it was decided to continue the round robin for the analysis of Benzene in accordance with the latest applicable version of the specification for Benzene: ASTM D2359.
In the interlaboratory study 51 laboratories in 22 different countries did register for participation. See appendix 2 for the number of participants per country. In this report, the results of the 2018 proficiency test for Benzene 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 tests (PT). Sample analyses for fit-for-use and homogeneity testing were subcontracted to an ISO/IEC 17025 accredited laboratory. It was decided to send one sample of Benzene (1 litre bottle, labelled #18020). The participants were requested to report rounded and unrounded test results. The unrounded test results were preferably used for statistical evaluation.

2.1   ACCREDITATION

The Institute for Interlaboratory Studies in Spijkenisse, the Netherlands, is accredited in agreement with ISO/IEC 17043:2010 (R007), since January 2000, by the Dutch Accreditation Council (Raad voor Accreditatie). This PT falls under the accredited scope. This ensures strict adherence to protocols for sample preparation and statistical evaluation and 100% confidentiality of participant's data. Feedback from the participants on the reported data is encouraged and customer's satisfaction is measured on regular basis by sending out questionnaires.

2.2   PROTOCOL

The protocol followed in the 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 March 2017 (iis-protocol, version 3.4). 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

The necessary bulk material of Benzene was a mixture of retained material. The approximately 70 kg of Benzene, after homogenisation, was filled into 68 amber glass bottles of 1 litre and labelled #18020. The homogeneity of the subsamples #18020 was checked by determination of Density at 20°C in accordance with ISO12185, Toluene in accordance with ASTM D4492 and Total Nitrogen in accordance with ASTM D6069 on 8 stratified randomly selected samples.

	Density at 20°C in kg/L	Toluene in mg/kg	Total Nitrogen in mg/kg
sample #18020-1	0.87897	331	0.64
sample #18020-2	0.87896	323	0.62
sample #18020-3	0.87896	316	0.61
sample #18020-4	0.87897	315	0.61
sample #18020-5	0.87897	313	0.61
sample #18020-6	0.87897	314	0.61
sample #18020-7	0.87897	316	0.61
sample #18020-8	0.87897	307	0.60

Table 1: homogeneity test results of Benzene subsamples #18020

From the above test results the repeatabilities were calculated and compared with 0.3 times the corresponding reproducibilities of the reference test methods in agreement with the procedure of ISO 13528, Annex B2 in the next table:

	Density at 20°C in kg/L	Toluene in mg/kg	Total Nitrogen in mg/kg
r (observed)	0.00001	20.2	0.03
Reference test method	ISO12185:96	ASTM 4492:10	ASTM D7184:15
0.3*R (reference test method)	0.00015	44.3	0.12

Table 2: evaluation of repeatabilities of subsamples #18020

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

To each of the participating laboratories one 1 litre bottle of Benzene labelled #18020 was sent on February 14, 2018. An SDS was added to the sample package.

2.5 STABILITY OF THE SAMPLES

The stability of Benzene, packed in amber glass bottles, was checked. The material was found sufficiently stable for the period of the proficiency test.

2.6 ANALYSES

The participants were requested to determine on sample #18020: Acid Wash Color, Acidity, Appearance, Bromine Index, Total Chlorides, Organic Chlorides, Color Pt/Co, Density at 20°C, Distillation, Total Nitrogen, Purity, Methylcyclohexane, Toluene, Nonaromatics, 1,4-Dioxane, Solidification Point, Sulphur and Thiophene.

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 calculations.

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 reanalysis). Additional or corrected test results are used for data analysis and the original test results are placed under 'Remarks' in the test result tables in appendix 1. Test results that came in after the deadline were not taken into account in this screening for suspect data and thus these participants were not requested for checks.

3.1 STATISTICS

The protocol followed in the 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 March 2017 (iis-protocol, version 3.4).

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 ISO 5725 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. When the uncertainty passed the evaluation no remarks are made in the report. However, when the uncertainty failed the evaluation it is mentioned in the report and it will have consequences for the evaluation of the test results.

Finally, the reproducibilities were calculated from the standard deviations by multiplying these 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 analysis 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 standard. 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. Therefore, the usual interpretation of z-scores is as follows:

$$|z| < 1 \quad \text{good}$$
$$1 < |z| < 2 \quad \text{satisfactory}$$
$$2 < |z| < 3 \quad \text{questionable}$$
$$3 < |z| \quad \text{unsatisfactory}$$

4   EVALUATION

In this interlaboratory study, no problems were encountered with dispatch of the samples. Eight reported the test results after the final reporting date and all laboratories reported one or more test results. Not all laboratories were able to perform all analyses requested. Finally, in total 545 numerical test results were reported by 51 participants. Observed were 24 outlying results, which is 4.4% 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, 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 methods are also in the tables together with the original data. The abbreviations, used in these tables, are listed in appendix 3.

Unfortunately, a suitable standard test method, providing the precision data, is not available for all determinations. For the tests, that have no available precision data, the calculated reproducibility was compared against the reproducibility estimated from the Horwitz equation.

In the iis PT reports, ASTM methods are referred to with a number (e.g. D5808) and an added designation for the year that the method was adopted or revised (e.g. D5808:09a). If applicable, a designation in parentheses is added to designate the year of reapproval (e.g. D5808:09a(2014)). In the results tables of Appendix 1 only the method number and year of adoption or revision e.g. D5808:09a will be used.

Acid Wash Color: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in good agreement with the requirements of ASTM D848:14.
For the statistical analysis, a result expressed as y- or y+ was changed into a numerical value as follows: y- changed into y-0.25 and y+ into y+0.25.

Acidity: This determination was not problematic. The majority of laboratories report "no free acid" (NFA) or "Pass" in accordance with ASTM D847:15.

Appearance: No analytical problems were observed. All labs agreed about the appearance of the sample, which was bright, clear and free of suspended matter (Pass).

Bromine Index: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D5776:14a.

Total Chlorides: This determination was problematic. No statistical outliers were observed. The calculated reproducibility is not in agreement with the requirements of ASTM D5194:18.
The possible cause of the large variation may be the low number of test results reported.

Organic Chlorides: This determination was not problematic. One statistical outlier was observed. The calculated reproducibility after rejection of the statistical outlier is in agreement with the requirements of ASTM D5808:09a(2014).

Color Pt/Co: This determination was not problematic. Three statistical outliers were observed. However, the calculated reproducibility after rejection of the statistical outliers is in agreement with the requirements of ASTM D1209:05e1(2011) and of ASTM D5386:16.

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

Distillation: This determination was not problematic. In total four statistical outliers were observed and one test result was excluded. However, all calculated reproducibilities after rejection of the suspect data are in agreement with the requirements of ASTM D850:16.
From the reported results of the 50% recovered, it appears that one participant probably did not correct the results for barometric pressure and thermometer inaccuracy as described in ASTM D850 (paragraph 11).

Total Nitrogen: 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 D4629:17.

Purity: This determination was problematic. Four statistical outliers were observed. The calculated reproducibility after rejection of the statistical outliers is not in agreement with the requirements of ASTM D4492:10 (this method was withdrawn in 2018).

Methylcyclohexane: This determination may be problematic. Two statistical outliers were observed. The calculated reproducibility after rejection of the statistical outliers is not agreement with the estimated reproducibility calculated using the Horwitz equation.
It is remarkable that the majority of the reporting laboratories used ASTM D4492, a method which may not be applicable for the determination of Methylcyclohexane, while only seven laboratories used ASTM D5713 that is suitable for the determination of Methylcyclohexane in Benzene.

Toluene: This determination was problematic for a number of laboratories. Four statistical outliers were observed. However, the calculated reproducibility after rejection of the statistical outliers is in good agreement with the requirements of ASTM D4492:10.

Nonaromatics: This determination was problematic. Two statistical outliers were observed. However, the calculated reproducibility after rejection of the statistical outliers is not in agreement with the requirements of ASTM D4492:10.

1,4-Dioxane: Twenty-two test results were reported. The participants agreed that the sample was not positive for 1,4-Dioxane (<10 mg/kg).

Solidification Point: This determination was not problematic. One statistical outlier was observed. However, the calculated reproducibility after rejection of the statistical outlier is in agreement with the requirements of ASTM D852:16.

Sulphur: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D5453:16e1.

Thiophene: Ten test results were reported. The participants agreed that the sample was low on Thiophene (<1 mg/kg).

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 average results, calculated reproducibilities and reproducibilities derived from literature standards (in casu ASTM, ISO standards) are compared in the next tables.

Parameter	unit	n	Average	2.8 *sd	R (lit)
Acid Wash Color		38	0.7 (1-)	0.6	2.0
Acidity	mg NaOH/100ml	37	No free acid	n.a.	n.a.
Appearance		45	Pass (C&B)	n.a.	n.a.
Bromine Index	mg Br/100g	39	1.7	2.7	4.6
Total Chlorides	mg/kg	6	1.11	1.11	0.9
Organic Chlorides	mg/kg	19	1.16	0.61	1.3
Color Pt/Co		35	5.1	3.5	7
Density at 20°C	kg/L	43	0.8790	0.0002	0.0005
Distillation, IBP	°C	33	79.8	0.3	0.4
Distillation, 50% rec.	°C	33	80.1	0.1	0.4
Distillation, DP	°C	31	80.3	0.2	0.4
Total Nitrogen	mg/kg	30	0.78	0.45	0.68
Purity	%M/M	43	99.963	0.011	0.006
Methylcyclohexane	mg/kg	25	8.5	5.1	2.8
Toluene	mg/kg	43	294.0	67.9	136.9
Nonaromatics	mg/kg	44	72.2	45.1	31.5
1,4-Dioxane	mg/kg	22	<10	n.a.	n.a.
Solidification Point	°C	25	5.48	0.04	0.05
Sulphur	mg/kg	25	0.53	0.35	0.36

Table 3: reproducibilities of tests on sample #18020

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

4.3   COMPARISON OF THE PROFICIENCY TEST OF MARCH 2018 WITH PREVIOUS PTS

	March 2018	March 2017	March 2016	Feb 2015	Feb 2014
Total Number of reporting labs	51	67	59	51	58
Number of results reported	545	743	793	729	800
Statistical outliers	24	32	19	15	36
Percentage outliers	4.4%	4.3%	2.4%	2.1%	4.5%

Table 4: comparison with previous proficiency tests.

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

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

	March 2018	March 2017	March 2016	Feb 2015	Feb 2014
Acid Wash Color	++	++	++	++	n.e.
Acidity	n.e.	n.e.	n.e.	n.e.	n.e.
Appearance	n.e.	n.e.	n.e.	n.e.	n.e.
Bromine Index	++	++	++	+	+
Total Chlorides	-	+/-	+	+	++
Organic Chlorides	++	+	++	++	++
Color Pt/Co	++	++	++	++	++
Density at 20°C	++	++	++	++	++
Distillation	++	++	++	++	+
Total Nitrogen	+	+/-	--	-	-
Purity	-	+/-	-	+/-	--
Methylcyclohexane	--	+/-	+/-	n.e.	n.e.
Toluene	++	++	++	+	++
Nonaromatics	-	-	+/-	-	+
1,4-Dioxane	n.e.	n.e.	n.e.	n.e.	n.e.
Solidification Point	+/-	+	+/-	+/-	--
Sulphur	+/-	n.e.	n.e.	n.e.	n.e.

Table 5: comparison determinations against the reference test methods

The performance of the determinations against the requirements of the respective reference test methods is listed in the above table. The following performance categories were used:
- ++:   group performed much better than the reference test method
- + :   group performed better than the reference test method
- +/-:   group performance equals the reference test method
- - :   group performed worse than the reference test method
- -- :   group performed much worse than the reference test method
- n.e.:   not evaluated

APPENDIX 1

Determination of Acid Wash Color (acid layer) on sample #18020

lab	method	value *)	mark	z(targ)	remarks
52	D848	0+		-0.67	
150	D848	0+		-0.67	
174	D848	1-		0.02	
311	D848	0+		-0.67	
317		-----		-----	
323	D848	-1		0.02	
334		-----		-----	
347		-----		-----	
357	D848	1-		0.02	
402	D848	1-		0.02	
444		-----		-----	
445	D848	1-		0.02	
551	D848	1-		0.02	
555	D848	1-		0.02	
663	D848	No. 1		0.36	
704	D848	1		0.36	
823	D848	1-		0.02	
852	D848	No.1-		0.02	
855	D848	No.1-		0.02	
862	D848	NO.1-		0.02	
864	D848	No.1-		0.02	
866	D848	NO.1-		0.02	
868	D848	No.1-		0.02	
870	D848	No.1-		0.02	
912	D848	1		0.36	
913	D848	Less Than 1.0		0.02	
962	D848	-1		0.02	
963	D848	1-		0.02	
1040		-----		-----	
1041	D848	1-		0.02	
1067	D848	1-		0.02	
1081		-----		-----	
1117		-----		-----	
1151		-----		-----	
1201	D848	1-		0.02	
1261	D848	1-		0.02	
1264	D848	1		0.36	
1294	D848	1		0.36	
1320		-----		-----	
1429	D848	1-		0.02	
1434	D848	0		-1.01	
1508		-----		-----	
1530	D848	1		0.36	
1538	D848	1		0.36	
1669		-----		-----	
1790		-----		-----	
1823		-----		-----	
1880	D848	<1		0.02	
1954	D848	<1		0.02	
6134	D848	0.8		0.08	
9008	D848	-1		0.02	

normality	not OK	
n	38	
outliers	0	
mean (n)	0.74 (1-)	
st.dev. (n)	0.217	
R(calc.)	0.61	
st.dev.(D848:14)	0.729	
R(D848:14)	2.04	

*) In the calculation of the mean, standard deviation, reproducibility and in the graphs, a reported value of 'y-', '-y' or '<y' is changed into y-0.25 (for example 1- into 0.75) and 'y+' is changed into y+0.25 (for example 0+ into 0.25).

Kernel Density
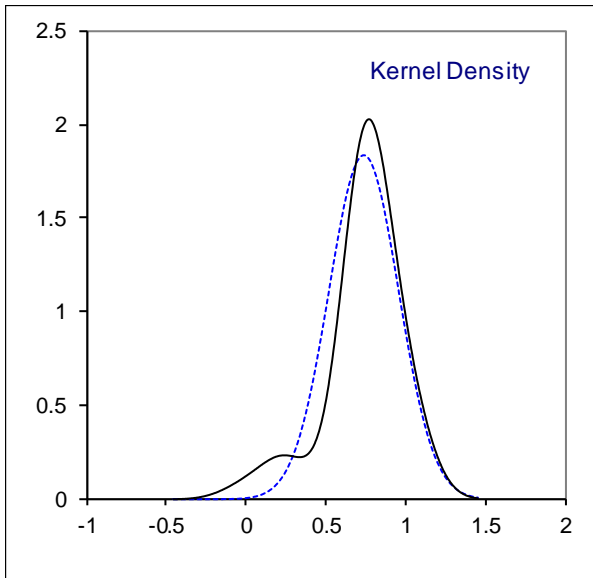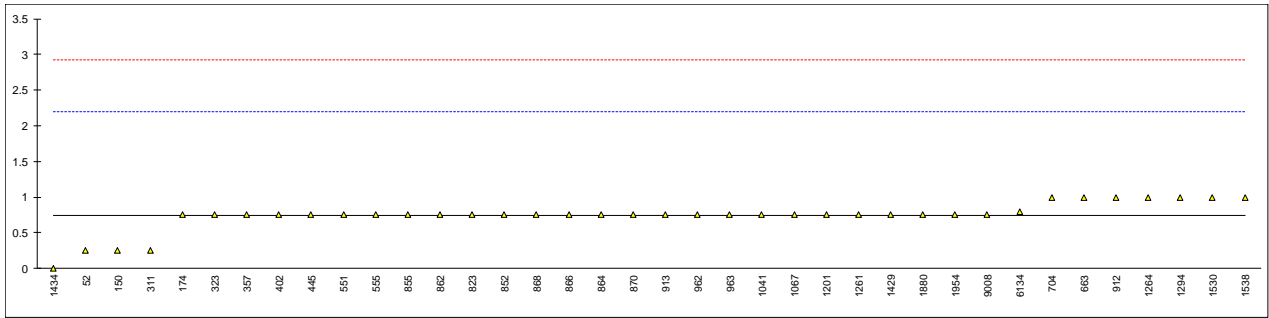
Determination of Acidity on sample #18020; results in mg NaOH/100mL

lab	method	value	mark	z(targ)	remarks
52	D847	Nil		-----	
150	D847	No Free Acid		-----	
174	D847	No Free Acid		-----	
311	D847	pass		-----	
317		-----		-----	
323	D847	no free acid		-----	
334		-----		-----	
347	D847	Pass		-----	
357	D847	No free acid		-----	
402	D847	pass		-----	
444		-----		-----	
445	D847	Pass		-----	
551	D847	Pass		-----	
555		-----		-----	
663	D847	Pass		-----	
704	D847	Pass		-----	
823	D847	no free acid		-----	
852	D847	No Free Acid		-----	
855	D847	No free acid		-----	
862	D847	No free acid		-----	
864	D847	No free acid		-----	
866	D847	NO FREE ACID		-----	
868	D847	PASS		-----	
870	D847	No Free Acid		-----	
912	D847	NO FREE ACID		-----	
913	D847	NIL		-----	
962	D847	nil		-----	
963	D847	No Free Acid		-----	
1040		-----		-----	
1041		-----		-----	
1067	D847	Pass		-----	
1081		-----		-----	
1117	D847	0.0952		-----	
1151		-----		-----	
1201	D847	passes		-----	
1261	D847	NFA		-----	
1264	D847	No Free Acid		-----	
1294	D847	NIL		-----	
1320		-----		-----	
1429		-----		-----	
1434	D847	negative		-----	
1508	D847	0		-----	
1530		-----		-----	
1538	D847	NFA		-----	
1669		-----		-----	
1790		-----		-----	
1823	D847	Pass		-----	
1880	D847	NFA		-----	
1954	D847	ND		-----	
6134	D847	No free acid		-----	
9008	D847	NFA		-----	
	n	37			
	mean (n)	No free acid			

Abbreviation
NFA = No free acid

Determination of Appearance on sample #18020

lab	method	value	mark	z(targ)	remarks
52	D4176	Pass		-----	
150	E2680	Clear and Bright		-----	
174	Visual	Clear & Free		-----	
311	INH-402	bright & clear		-----	
317	D4176	Pass		-----	
323	E2680	pass		-----	
334		-----		-----	
347	E2680	Pass		-----	
357	E2680	Pass		-----	
402	Visual	pass		-----	
444	Visual	Pass		-----	
445	D4176	Pass		-----	
551	D4176	Pass test		-----	
555	Visual	Clear and free from impurities		-----	
663	Visual	Bright and Clear		-----	
704	E2680	Pass		-----	
823	E2680	Pass		-----	
852	Visual	pass		-----	
855	E2680	Pass		-----	
862	E2680	PASS		-----	
864	D4176	Pass		-----	
866	E2680	Pass		-----	
868	E2680	PASS		-----	
870	E2680	Pass		-----	
912	E2680	PASS		-----	
913	E2680	CFSM		-----	
962	D4176	Pass		-----	
963	E2680	Pass		-----	
1040	Visual	clear, bright		-----	
1041		-----		-----	
1067	Visual	Clear and Bright		-----	
1081		-----		-----	
1117	D4176	PASS		-----	
1151		-----		-----	
1201	D4176	Clear and Bright		-----	
1261	Visual	Clear and Bright		-----	
1264	Visual	Clear and Bright		-----	
1294	Visual	CLEAR		-----	
1320		-----		-----	
1429	E2680	Pass		-----	
1434	Visual	clear liq		-----	
1508	Visual	Clear		-----	
1530	D4176	pass		-----	
1538	Visual	C&B		-----	
1669	Visual	Claro y Brillante		-----	
1790		-----		-----	
1823	D4176	Clear/FFSM/No free water		-----	
1880	Visual	Pass		-----	
1954	Visual	CLEAR		-----	
6134	Visual	CLEAR AND BRIGHT		-----	
9008		Clear Liquid		-----	

n	45
mean (n)	Pass (Clear and bright)

Abbreviations:
C&B / B&C   = clear and bright / bright and clear
CFSM   = clear and free from suspended matter
FFSM   = free from suspended matter

Determination of Bromine Index on sample #18020; results in mg Br/100g

lab	method	value	mark	z(targ)	remarks
52		-----		-----	
150	D1492	1		-0.43	
174		-----		-----	
311	D5776	1.0		-0.43	
317	D5776	1.0		-0.43	
323	D5776	1.0		-0.43	
334	D5776	1.2		-0.31	
347		-----		-----	
357	D5776	3.9		1.33	
402	D5776	0.7		-0.61	
444	D5776	1.24		-0.28	
445	D1492	3.1		0.85	
551	D5776	0.9		-0.49	
555	D5776	1.9475		0.15	
663	D5776	1.8		0.06	
704	D5776	1.38		-0.20	
823		-----		-----	
852	D5776	1.4		-0.19	
855	D5776	1.5		-0.13	
862	D5776	1.4		-0.19	
864	D5776	1.5		-0.13	
866	D5776	1.5		-0.13	
868	D5776	<10		-----	
870	D5776	1.5		-0.13	
912		-----		-----	
913	D5776	<0.5		-----	
962		-----		-----	
963		-----		-----	
1040	D5776	1.40		-0.19	
1041	DIN51774	1.37		-0.21	
1067	D2710	< 10		-----	
1081	D1492	4.33520		1.60	
1117	D1492	1.8		0.06	
1151		-----		-----	
1201		-----	W	-----	first reported: 20.5 according to ASTM D2710
1261	D1492	1.7		0.00	
1264	D1492	1.40		-0.19	
1294	D1492	3.88		1.32	
1320	D1492	2.1		0.24	
1429	D2710	1.0		-0.43	
1434	D5776	0.37		-0.81	
1508	D2710	0.25		-0.89	
1530	D1492	1		-0.43	
1538	D1492	3.49		1.09	
1669	D5776	2.0		0.18	
1790	D5776	1.31		-0.24	
1823	D1492	1.13		-0.35	
1880	D1492	2.5		0.48	
1954	D2710	2.36		0.40	
6134	D5776	1.1233		-0.36	
9008	D1492	3.1		0.85	
	normality	not OK			
	n	39			
	outliers	0			
	mean (n)	1.71			
	st.dev. (n)	0.967			
	R(calc.)	2.71			
	st.dev.(D5776:14a)	1.643			
	R(D5776:14a)	4.6			

Kernel Density
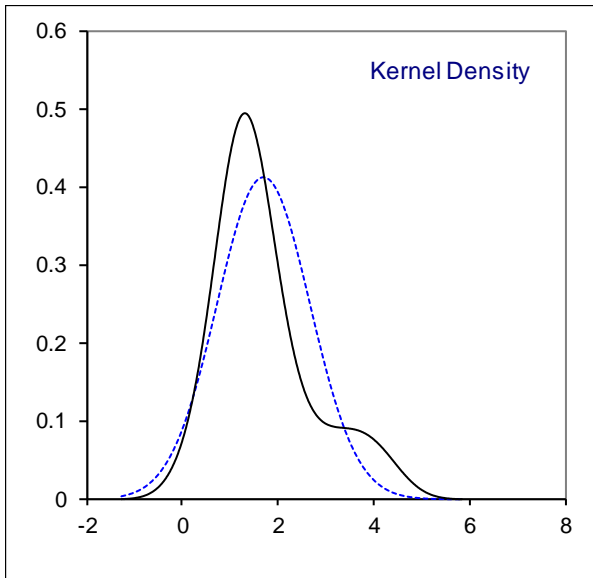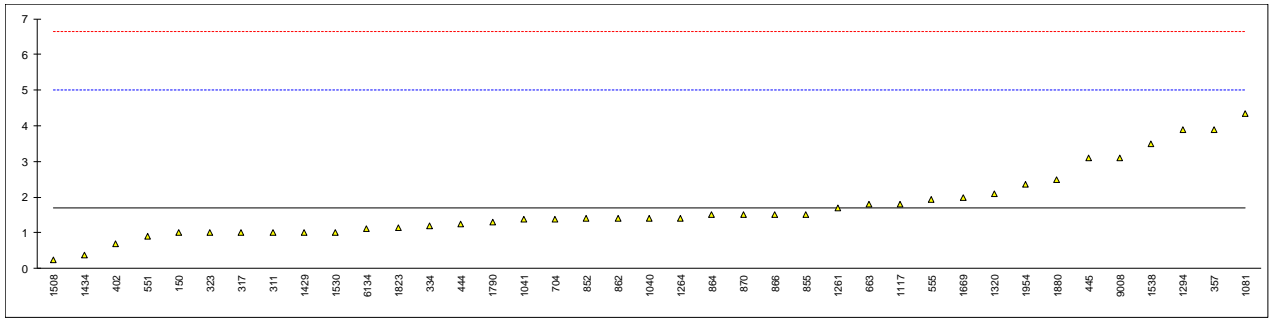
Determination of Chlorides, Total on sample #18020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52		-----		-----	
150	D7359	1.2		0.27	
174		-----		-----	
311		-----		-----	
317		-----		-----	
323		-----		-----	
334		0.8		-0.97	
347		-----		-----	
357		-----		-----	
402		-----		-----	
444		-----		-----	
445		-----		-----	
551		-----		-----	
555		-----		-----	
663		-----		-----	
704	UOP588	<1		-----	
823		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1040		-----		-----	
1041		-----		-----	
1067		-----		-----	
1081		-----		-----	
1117		-----		-----	
1151	D7536	1.59	C	1.49	first reported: 3.17
1201		-----		-----	
1261		-----		-----	
1264		-----		-----	
1294		-----		-----	
1320		-----		-----	
1429	D7359	1.1		-0.04	
1434	D7359	0.53		-1.81	
1508		-----		-----	
1530		-----		-----	
1538		-----		-----	
1669		-----		-----	
1790		-----		-----	
1823		-----		-----	
1880	D7359	1.45		1.05	
1954		-----		-----	
6134		-----		-----	
9008		-----		-----	

normality	unknown
n	6
outliers	0
mean (n)	1.112
st.dev. (n)	0.3967
R(calc.)	1.111
st.dev.(D5194:18)	0.3214
R(D5194:18)	0.9
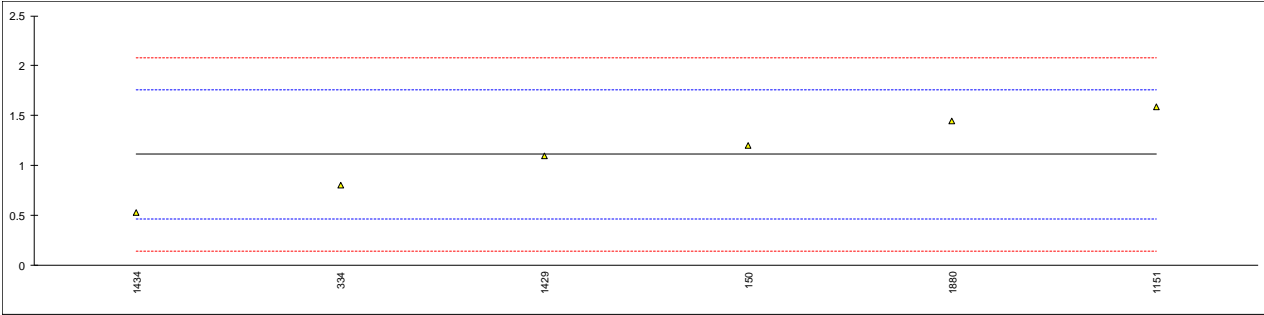
Determination of Chlorides, Organic on sample #18020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52		-----		-----	
150	D7359	1.2		0.08	
174		-----		-----	
311	D5808	1		-0.35	
317	UOP779	1.3		0.30	
323	D5808	2	R(0.05)	1.81	
334	D5808	1.40		0.51	
347		-----		-----	
357		-----		-----	
402	D5808	<1		-----	
444	IP510	1.2		0.08	
445	IP510	<2		-----	
551		-----		-----	
555		-----		-----	
663		-----		-----	
704	UOP588	<1		-----	
823		-----		-----	
852	D5808	1.1		-0.13	
855	D5808	1.3		0.30	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868	D5808	1.0		-0.35	
870		-----		-----	
912	D5808	1.3		0.30	
913		-----		-----	
962		-----		-----	
963	D5808	0.67		-1.06	
1040	EN14077	1.42		0.56	
1041		-----		-----	
1067	UOP779	1.1		-0.13	
1081	D5808	1.060		-0.22	
1117		-----		-----	
1151		-----		-----	
1201	D5808	1.0		-0.35	
1261		-----		-----	
1264		-----		-----	
1294		-----		-----	
1320	EN14077	1.13		-0.07	
1429		-----		-----	
1434		-----		-----	
1508		-----		-----	
1530		-----		-----	
1538	D5808	1.21		0.10	
1669		-----		-----	
1790		-----		-----	
1823		-----		-----	
1880		-----		-----	
1954	D5808	0.84		-0.69	
6134	D4929B	1.64		1.03	
9008	D5808	1.2		0.08	
	normality	OK			
	n	19			
	outliers	1			
	mean (n)	1.162			
	st.dev. (n)	0.2185			
	R(calc.)	0.612			
	st.dev.(D5808:09a)	0.4643			
	R(D5808:09a)	1.3			

Kernel Density
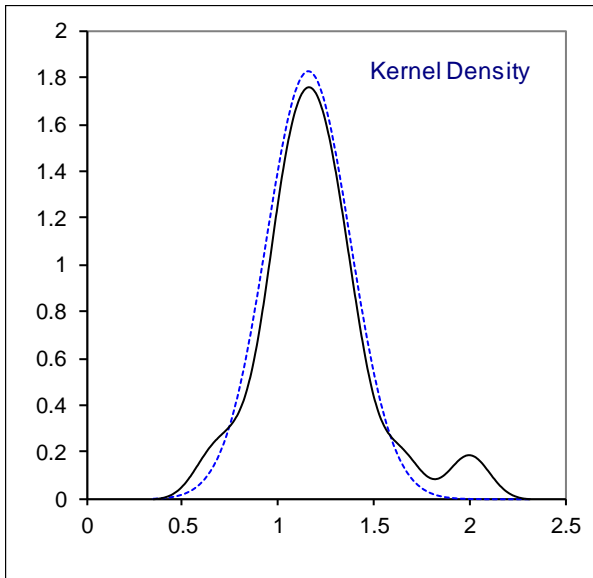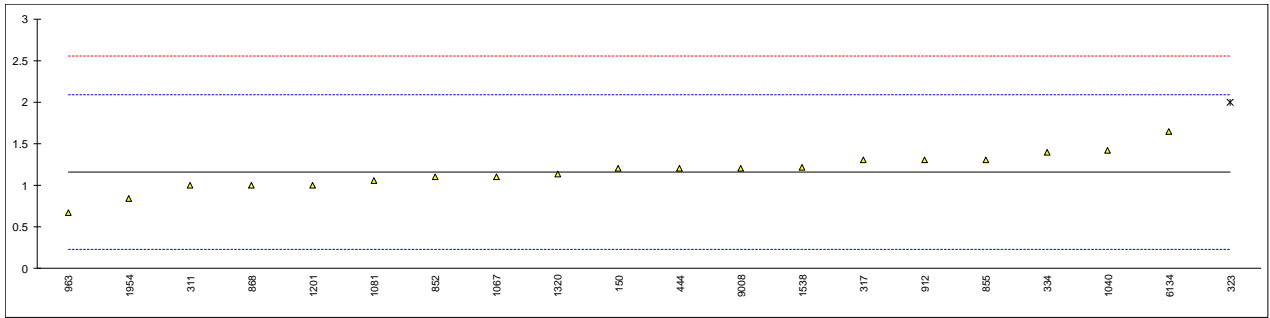
Determination of Color Pt/Co on sample #18020

lab	method	value	mark	z(targ)	remarks
52	D5386	5.9		0.31	
150	D5386	6		0.35	
174	D1209	7		0.75	
311	D1209	5		-0.05	
317	D1209	5		-0.05	
323	D1209	5		-0.05	
334		-----		-----	
347	D5386	3		-0.85	
357	D5386	6		0.35	
402	D1209	5		-0.05	
444	D5386	6		0.35	
445	D1209	4.7		-0.17	
551	D1209	4		-0.45	
555	D1209	4		-0.45	
663	D1209	5		-0.05	
704	D1209	5		-0.05	
823	D5386	6.6		0.59	
852	D1209	5		-0.05	
855	D1209	<5		-----	
862	D1209	<5		-----	
864	D1209	<5		-----	
866	D1209	2		-1.25	
868	D1209	5		-0.05	
870	D1209	4		-0.45	
912		-----		-----	
913	D5386	3.6		-0.61	
962	D1209	4		-0.45	
963	D1209	4		-0.45	
1040	ISO6271	<5		-----	
1041		-----		-----	
1067	D1209	< 5		-----	
1081	D5386	5		-0.05	
1117	D1209	6		0.35	
1151		-----		-----	
1201	D1209	7		0.75	
1261	D5386	6		0.35	
1264	D1209	5		-0.05	
1294	D1209	<10		-----	
1320	D1209	5		-0.05	
1429	D1209	< 5		-----	
1434	D1209	10	R(0.05)	1.95	
1508	D1209	0	R(0.05)	-2.05	
1530	D1209	<5		-----	
1538	D1209	3		-0.85	
1669		-----		-----	
1790	D1209	0	R(0.05)	-2.05	
1823	D5386	6.7		0.63	
1880	D5386	7.30		0.87	
1954	D1209	5		-0.05	
6134	D1209	5.5		0.15	
9008	D5386	7.2		0.83	
	normality	OK			
	n	35			
	outliers	3			
	mean (n)	5.13			
	st.dev. (n)	1.250			
	R(calc.)	3.50			
	st.dev.(D1209:05)	2.500			
	R(D1209:05)	7		compare R(D5386:16) = 5.39	

Kernel Density
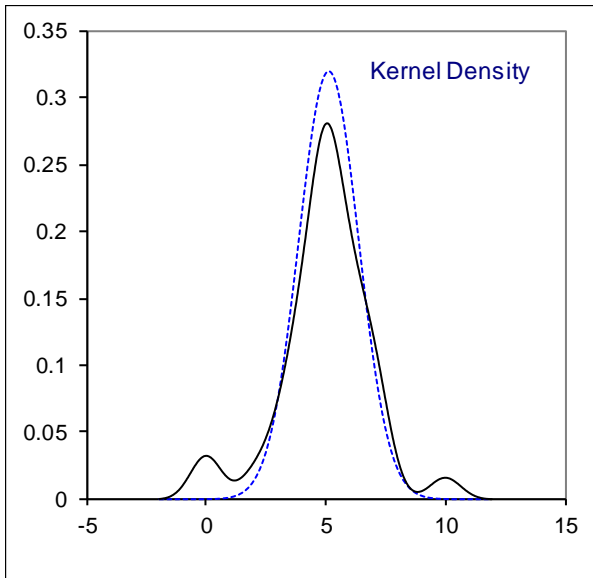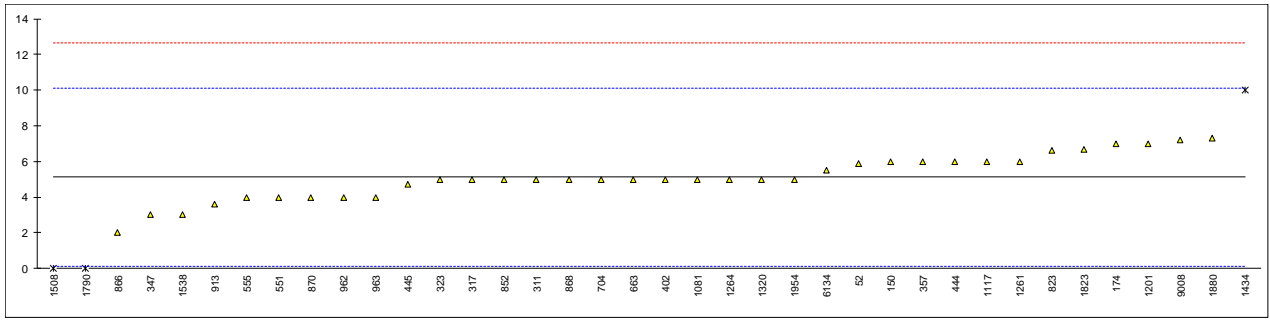
Determination of Density at 20°C on sample #18020; results in kg/L

lab	method	value	mark	z(targ)	remarks
52	D4052	0.8790		0.16	
150	D4052	0.8792	R(0.05)	1.28	
174	D4052	0.8790		0.16	
311	D4052	0.8790		0.16	
317	D4052	0.8790		0.16	
323	D4052	0.8789		-0.40	
334	ISO12185	0.8792	R(0.05)	1.28	
347	D4052	0.87896		-0.06	
357	D4052	0.87891		-0.34	
402	ISO12185	0.8790		0.16	
444	D4052	0.8791		0.72	
445	D4052	0.8790		0.16	
551	D4052	0.8790		0.16	
555	D4052	0.8789		-0.40	
663	D4052	0.87895		-0.12	
704	ISO12185	0.87898		0.05	
823	ISO12185	0.87900		0.16	
852	D4052	0.8790		0.16	
855	D4052	0.87902		0.27	
862	D4052	0.87901		0.22	
864	D4052	0.87902		0.27	
866	ISO12185	0.87906		0.50	
868	D4052	0.87902		0.27	
870	D4052	0.87904		0.38	
912	D4052	0.8790		0.16	
913	D4052	0.8789		-0.40	
962	D4052	0.8790		0.16	
963	D4052	0.8789		-0.40	
1040	ISO12185	0.8790		0.16	
1041		-----		-----	
1067	ISO12185	0.8790		0.16	
1081		-----		-----	
1117		-----		-----	
1151		-----		-----	
1201	D4052	0.8790		0.16	
1261	D4052	0.87901		0.22	
1264	D4052	0.87901		0.22	
1294	D4052	0.87887	C	-0.57	first reported: 0.88063 (at 15.56°C)
1320	ISO12185	0.8789		-0.40	
1429	D4052	0.8790		0.16	
1434	D4052	0.87892		-0.29	
1508		-----		-----	
1530	ISO12185	0.8790		0.16	
1538	ISO3675	0.879		0.16	
1669	D4052	0.8790		0.16	
1790		-----		-----	
1823	D4052	0.8788		-0.96	
1880	D4052	0.8789		-0.40	
1954	D4052	0.8789		-0.40	
6134	D4052	0.8789		-0.40	
9008	D4052	0.8789		-0.40	

|		
normality	OK	
n	43	
outliers	2	
mean (n)	0.87897	
st.dev. (n)	0.000059	
R(calc.)	0.00017	
st.dev.(ISO12185:96)	0.000179	
R(ISO12185:96)	0.0005	

Kernel Density
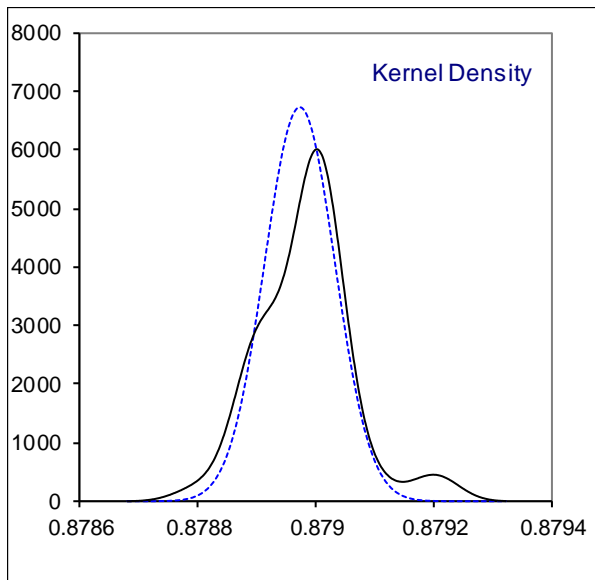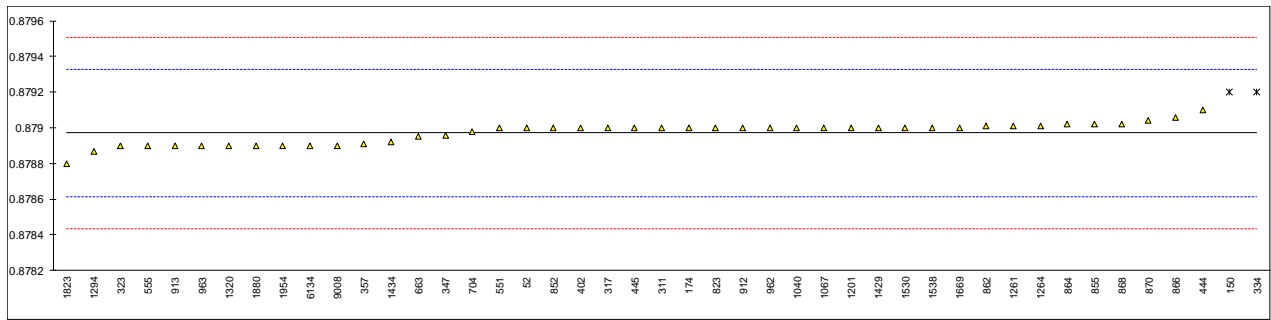
Determination of Distillation on sample #18020; results in °C

Lab	method	IBP	mark	z(targ)	50%	mark	z(targ)	DP	mark	z(targ)
52	D850-automated	79.7		-0.37	80.1		-0.04	80.4		0.71
150	D850-automated	79.7		-0.37	80.1		-0.04	80.3		0.04
174		79.7		-0.37	80.1		-0.04	80.2		-0.63
311	D850-automated	79.7		-0.37	80.1		-0.04	80.2		-0.63
317		-----		-----	-----		-----	-----		-----
323	D850-manual	79.8		0.30	80.1		-0.04	80.3		0.04
334		-----		-----	-----		-----	-----		-----
347		-----		-----	-----		-----	-----		-----
357	D850-automated	79.7		-0.37	80.1		-0.04	80.3		0.04
402	D850-manual	79.81		0.37	80.11		0.02	80.21		-0.56
444		-----		-----	-----		-----	-----		-----
445	D850-manual	79.9		0.97	80.1		-0.04	81.5	R(0.01)	8.04
551		-----		-----	-----		-----	-----		-----
555	D850	79.6		-1.03	80.2		0.62	81.2	R(0.01)	6.04
663	D850-automated	79.80		0.30	80.10		-0.04	80.30		0.04
704	D850-manual	79.8		0.30	80.1		-0.04	80.3		0.04
823		-----		-----	-----		-----	-----		-----
852	D850-manual	79.9		0.97	80.1		-0.04	80.3		0.04
855	D850-manual	79.8		0.30	80.1		-0.04	80.3		0.04
862	D850-manual	79.9		0.97	80.1		-0.04	80.3		0.04
864	D850-automated	79.8		0.30	80.1		-0.04	80.2		-0.63
866	D850-manual	79.7		-0.37	80.1		-0.04	80.3		0.04
868	D850-manual	79.8		0.30	80.1		-0.04	80.3		0.04
870	D850-manual	79.8		0.30	80.1		-0.04	80.2		-0.63
912	D850-manual	79.9		0.97	80.1		-0.04	80.5		1.37
913	D850-manual	79.7		-0.37	80.1		-0.04	80.3		0.04
962	D850-automated	79.6	C	-1.03	80.1	C	-0.04	80.3	C	0.04
963	D850-automated	79.6		-1.03	80.1		-0.04	80.3		0.04
1040		-----		-----	-----		-----	-----		-----
1041		-----		-----	-----		-----	-----		-----
1067	D850-manual	79.8		0.30	80.1		-0.04	80.4		0.71
1081		-----		-----	-----		-----	-----		-----
1117		-----		-----	-----		-----	-----		-----
1151		-----		-----	-----		-----	-----		-----
1201	D850-automated	79.7		-0.37	80.1		-0.04	80.3		0.04
1261	D850-automated	79.7		-0.37	80.1		-0.04	80.3		0.04
1264	D850-automated	79.8		0.30	80.1		-0.04	80.3		0.04
1294	D850-automated	79.6		-1.03	80.1		-0.04	80.3		0.04
1320		-----		-----	-----		-----	-----		-----
1429	D850-automated	79.8		0.30	80.1		-0.04	80.3		0.04
1434	D850-automated	79.7		-0.37	80.2		0.62	80.2		-0.63
1508		-----		-----	-----		-----	-----		-----
1530	D850-automated	80.3	R(0.01)	3.63	80.4	R(0.01)	1.96	80.5	ex	1.37
1538	D850-automated	79.9		0.97	80.1		-0.04	80.3		0.04
1669		-----		-----	-----		-----	-----		-----
1790		-----		-----	-----		-----	-----		-----
1823		-----		-----	-----		-----	-----		-----
1880	D850-automated	79.8		0.30	80.2		0.62	80.3		0.04
1954	D850-automated	79.6		-1.03	80.1		-0.04	80.2		-0.63
6134	D850-manual	79.8		0.30	80.0		-0.71	80.4		0.71
9008		-----		-----	-----		-----	-----		-----
	normality	OK			not OK			suspect		
	n	33			33			31		
	outliers	1			1			2 (+1ex)		
	mean (n)	79.75			80.11			80.29		
	st.dev. (n)	0.094			0.035			0.068		
	R(calc.)	0.26			0.097			0.19		
	st.dev.(D850:16)	0.150			0.150			0.150		
	R(D850:16)	0.42			0.42			0.42		

Lab 962 first reported for IBP:79.4, for 50% recovered: 79.9 and for Dry Point: 80.1
Lab 1530: test result for Dry Point is excluded, for the other two test results are outliers, this lab probably did not correct for barometric pressure and thermometer inaccuracy.

Theoretical mid-boiling point = 80.1°C
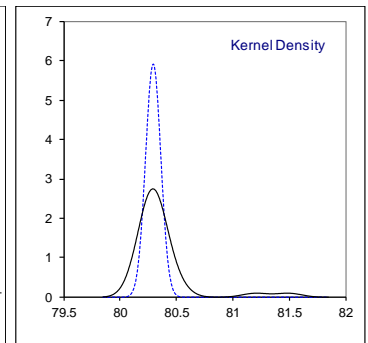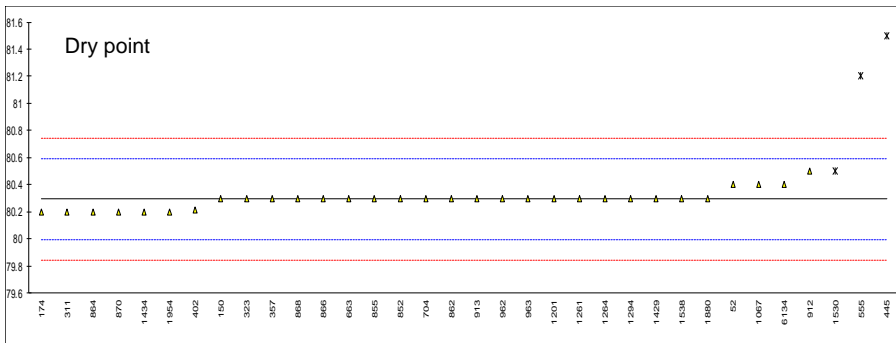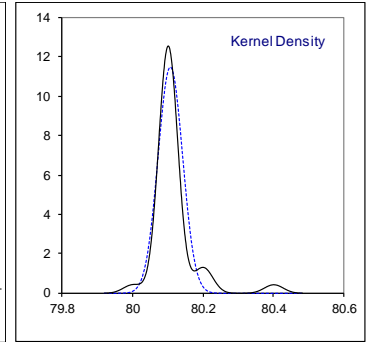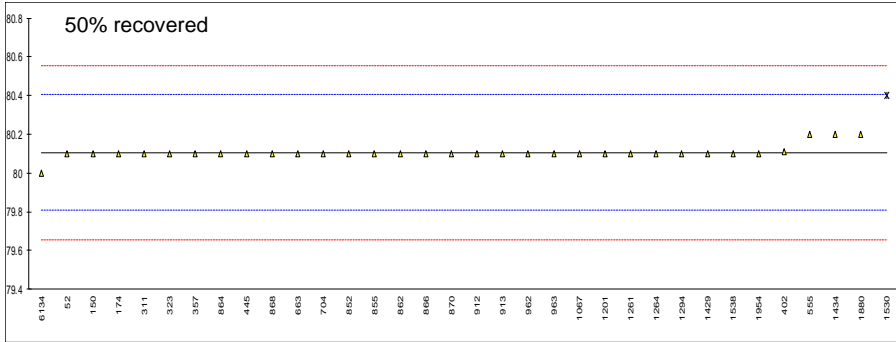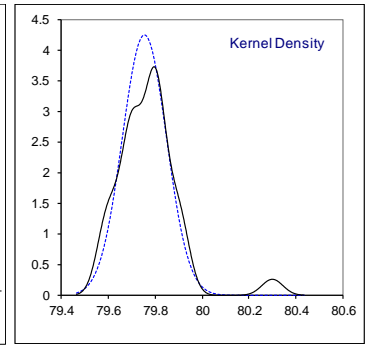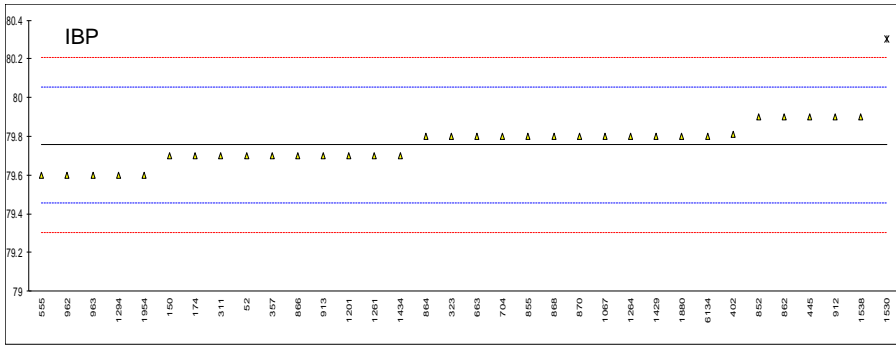
Determination of Total Nitrogen on sample #18020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7184	0.886		0.45	
150	D7184	0.57		-0.84	
174		-----		-----	
311	D6069	0.7		-0.31	
317	D4629	0.8		0.10	
323	D6069	< 1.0		-----	
334	D4629	0.5		-1.13	
347	D4629	0.76		-0.06	
357	D4629	0.8		0.10	
402	D4629	<0,3		-----	
444	D4629	0.746		-0.12	
445	D4629	0.94		0.68	
551	D4629	1.5	C,R(0.01)	2.98	first reported: 2.3
555		-----		-----	
663		-----		-----	
704	D4629	1.0		0.92	
823		-----		-----	
852		-----		-----	
855		-----		-----	
862	D6069	<1		-----	
864	D7184	<1		-----	
866		-----		-----	
868	D4629	0.7		-0.31	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1040	D7184	0.73		-0.19	
1041	D6069	0.62		-0.64	
1067	D6069	0.6		-0.72	
1081	D6069	0.85		0.31	
1117	D7184	0.955		0.74	
1151		-----		-----	
1201	D4629	0.4		-1.54	
1261		-----		-----	
1264	D7184	0.82		0.18	
1294	D6069	0.95		0.72	
1320	D6069	0.72		-0.23	
1429	D4629	< 0.3		-----	
1434	D7184	0.60868		-0.68	
1508		-----		-----	
1530	D6069	0.8		0.10	
1538	D7184	1.1		1.33	
1669	D4629	0.6		-0.72	
1790	D6069	0.855		0.33	
1823	D6069	0.88		0.43	
1880	D6069	0.88		0.43	
1954	D7184	0.76		-0.06	
6134	D6069	1.03		1.05	
9008	D6069	0.7		-0.31	
	normality	OK			
	n	30			
	outliers	1			
	mean (n)	0.775			
	st.dev. (n)	0.1615			
	R(calc.)	0.452			
	st.dev.(D4629:17)	0.2434			
	R(D4629:17)	0.682			Compare D7184:15: 0.3603 Range D7184: 0.1-1.2 mg/kg

Kernel Density
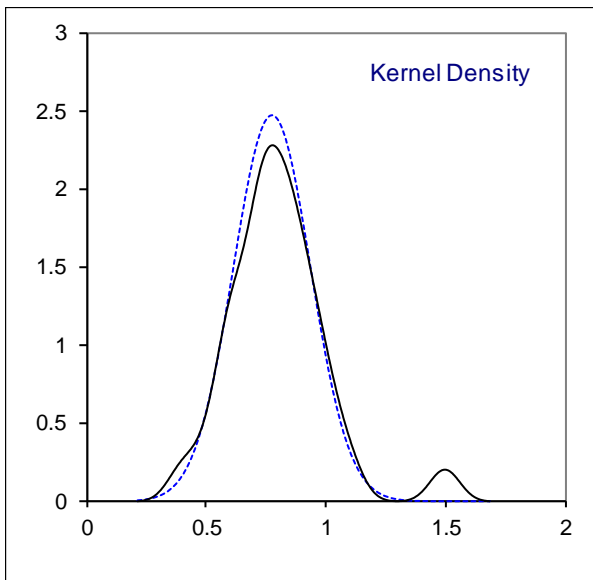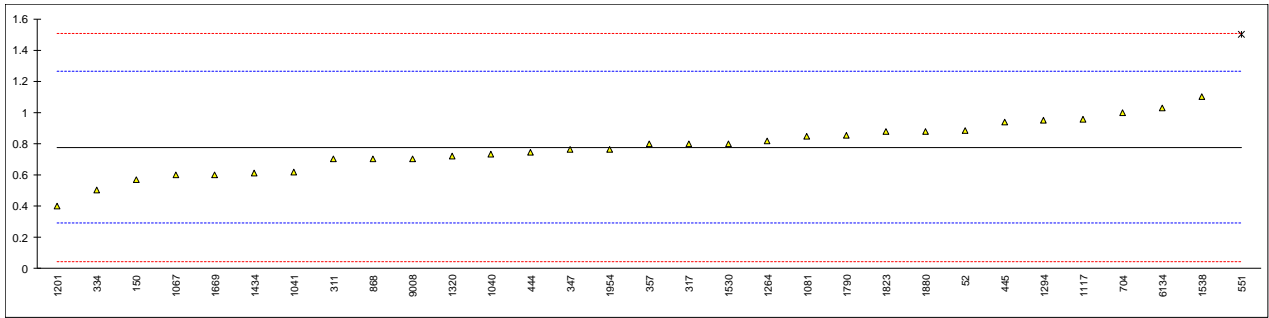
Determination of Purity by GC on sample #18020; results in %M/M

lab	method	value	mark	z(targ)	remarks
52	D7504	99.960		-1.31	
150	D4492	99.96		-1.31	
174		-----		-----	
311	D4492	99.96		-1.31	
317	D4492	99.97	C	3.26	first reported: 99.93
323	D7504	99.96		-1.31	
334	D4492	99.97		3.26	
347	D4492	99.963		0.06	
357	D4492	99.961		-0.85	
402	D4492	99.9574		-2.50	
444	D4492	99.9602		-1.22	
445	D4492	99.96		-1.31	
551	D4492	99.960		-1.31	
555	D4492	99.94	R(0.01)	-10.47	
663	D4492	99.968		2.35	
704	D4492	99.9577		-2.36	
823	D7360	99.9610		-0.85	
852	D4492	99.964		0.52	
855	D4492	99.963		0.06	
862	D4492	99.962		-0.40	
864	D4492	99.968		2.35	
866	D4492	99.96		-1.31	
868	D4492	99.962		-0.40	
870	D4492	99.965		0.98	
912		-----		-----	
913	D4492	99.97		3.26	
962		-----		-----	
963	D4492	99.96		-1.31	
1040	D7504	99.9605		-1.08	
1041	In house	99.9611	C	-0.81	first reported: 99.8811
1067	In house	99.97		3.26	
1081	D4492	99.96099		-0.86	
1117	D4492	99.96		-1.31	
1151		-----		-----	
1201	D4492	99.94	R(0.01)	-10.47	
1261	D4492	99.9631		0.11	
1264	D4492	99.964		0.52	
1294	D4492	99.962		-0.40	
1320	D4492	99.971		3.72	
1429	D4492	99.989	R(0.01)	11.96	
1434	D4492	99.96345		0.27	
1508	D2360	99.964		0.52	
1530	D4492	99.967		1.89	
1538	D4492	99.96		-1.31	
1669	D5713	99.97		3.26	
1790	D4492	99.9470	R(0.01)	-7.26	
1823	D4492	99.96		-1.31	
1880	D4492	99.963		0.06	
1954	D4492	99.9588		-1.86	
6134	D4492	99.96107		-0.82	
9008	D4492	99.961		-0.85	

	normality	OK	
	n	43	
	outliers	4	
	mean (n)	99.9629	
	st.dev. (n)	0.00377	
	R(calc.)	0.0106	
	st.dev.(D4492:10)	0.00219	
	R(D4492:10)	0.0061	

Kernel Density
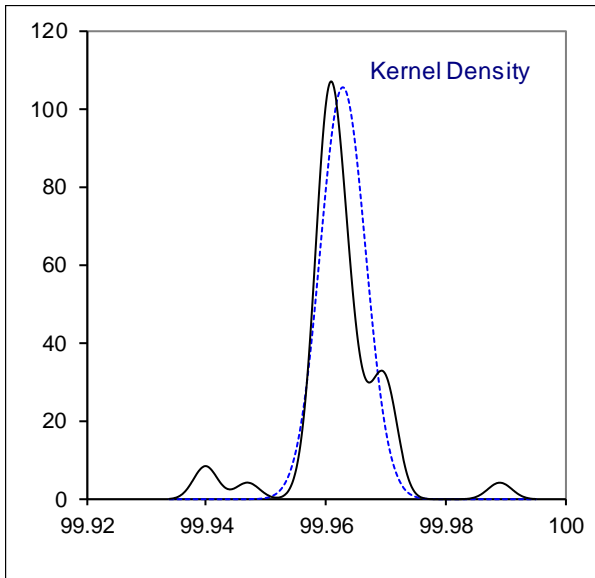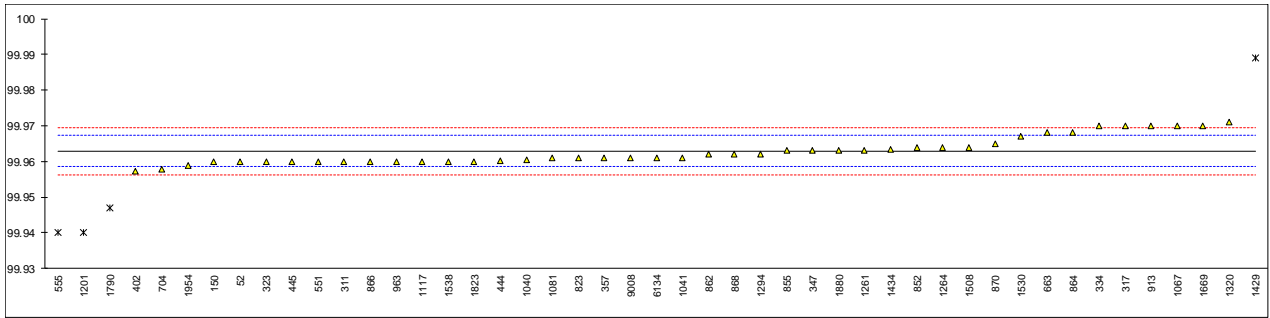
Determination of Methylcyclohexane on sample #18020 in mg/kg

lab	method	value	mark	z(targ)	remarks
52		-----		-----	
150	D5713	9		0.48	
174		-----		-----	
311	D5713	10		1.49	
317	D5713	<10		-----	
323	D5713	8		-0.53	
334	D4492	10	C	1.49	first reported: 0.001
347		-----		-----	
357	D4492	8		-0.53	
402	D4492	6.77		-1.78	
444	D4492	9		0.48	
445	D4492	8		-0.53	
551	D4492	12		3.52	
555		-----		-----	
663		-----		-----	
704		<10		-----	
823	D5713	9		0.48	
852	D4492	<10		-----	
855	D4492	<10		-----	
862	D4492	<10		-----	
864	D4492	<10		-----	
866	D4492	7.1		-1.44	
868	D4492	8.1		-0.43	
870	D4492	6		-2.55	
912		-----		-----	
913	D4492	ND[<5.0 ppm]		<-3.57	Possibly a false negative test result?
962		-----		-----	
963	D4492	18	R(0.01)	9.59	
1040	D7504	10.0		1.49	
1041		-----		-----	
1067	In house	10		1.49	
1081	D5713	9.57		1.06	
1117	D4492	10		1.49	
1151		-----		-----	
1201	D4492	5		-3.57	
1261		-----		-----	
1264	D4492	7		-1.54	
1294		-----		-----	
1320	D4492	3.95		-4.63	
1429	D4492	9		0.48	
1434	D4492	10.1		1.60	
1508		-----		-----	
1530	D4492	28	R(0.01)	19.72	
1538		-----		-----	
1669	D5713	8		-0.53	
1790	D4492	9		0.48	
1823		-----		-----	
1880		-----		-----	
1954	D4492	10.5		2.00	
6134		-----		-----	
9008		-----		-----	

normality	OK
n	25
outliers	2
mean (n)	8.52
st.dev. (n)	1.826
R(calc.)	5.11
st.dev.(Horwitz)	0.988
R(Horwitz)	2.77

Kernel Density
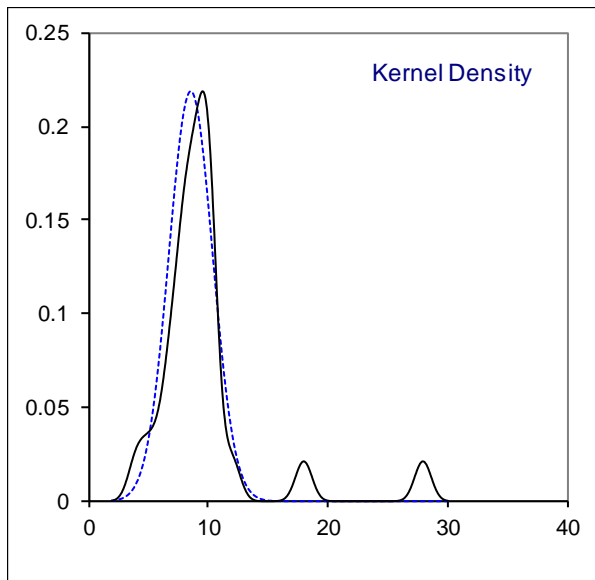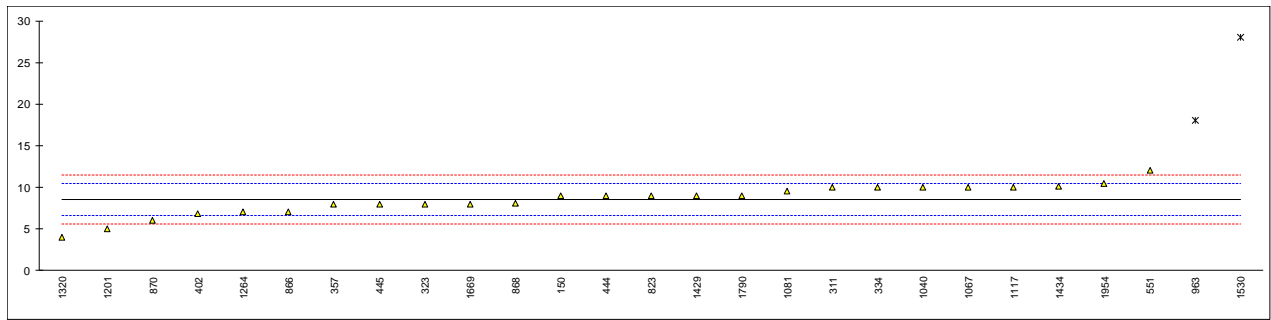
Determination of Toluene on sample #18020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7504	298		0.08	
150	D4492	300	C	0.12	first reported: 0.03
174		-----		-----	
311	D4492	320		0.53	
317	D4492	290		-0.08	
323	D7504	279		-0.31	
334	D4492	270	C	-0.49	first reported: 0.0270
347	D4492	289		-0.10	
357	D4492	320		0.53	
402	D4492	296.03		0.04	
444	D4492	301		0.14	
445	D4492	249		-0.92	
551	D4492	320		0.53	
555		-----		-----	
663	D4492	247.2		-0.96	
704	D4492	321		0.55	
823	D7360	295		0.02	
852	D4492	286		-0.16	
855	D4492	300		0.12	
862	D4492	300		0.12	
864	D4492	305		0.23	
866	D4492	290		-0.08	
868	D4492	290		-0.08	
870	D4492	282		-0.25	
912		-----		-----	
913	D4492	335		0.84	
962		-----		-----	
963	D4492	320		0.53	
1040	D7504	29.8	R(0.01)	-5.41	
1041	In house	286		-0.16	
1067	In house	280		-0.29	
1081	D4492	303.3519		0.19	
1117	D4492	300		0.12	
1151	In house	297.3	C	0.07	first reported: 405.71
1201	D4492	515	R(0.01)	4.52	
1261	D4492	286		-0.16	
1264	D4492	300		0.12	
1294	D4492	360	C	1.35	first reported: 0.0360
1320	D4492	254.70		-0.80	
1429	D4492	27	R(0.01)	-5.46	
1434	D4492	304.4	C	0.21	first reported: 30.44
1508	D2360	220	C	-1.51	first reported: 256
1530	D4492	283		-0.22	
1538	D4492	301		0.14	
1669	D5713	257	C	-0.76	first reported: 2.57
1790	D4492	430	R(0.01)	2.78	
1823	D4492	302		0.16	
1880	D4492	290		-0.08	
1954	D4492	311.6		0.36	
6134	D4492	301.6		0.16	
9008	D4492	300		0.12	

	normality	not OK
	n	43
	outliers	4
	mean (n)	293.98
	st.dev. (n)	24.256
	R(calc.)	67.92
	st.dev.(D4492:10)	48.876
	R(D4492:10)	136.85

Kernel Density
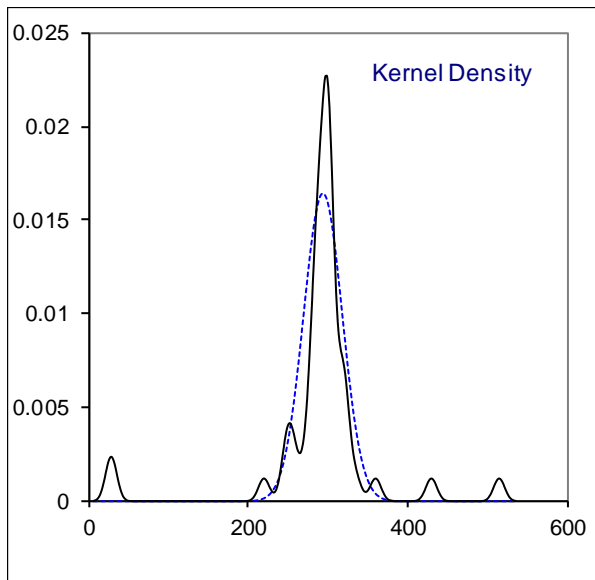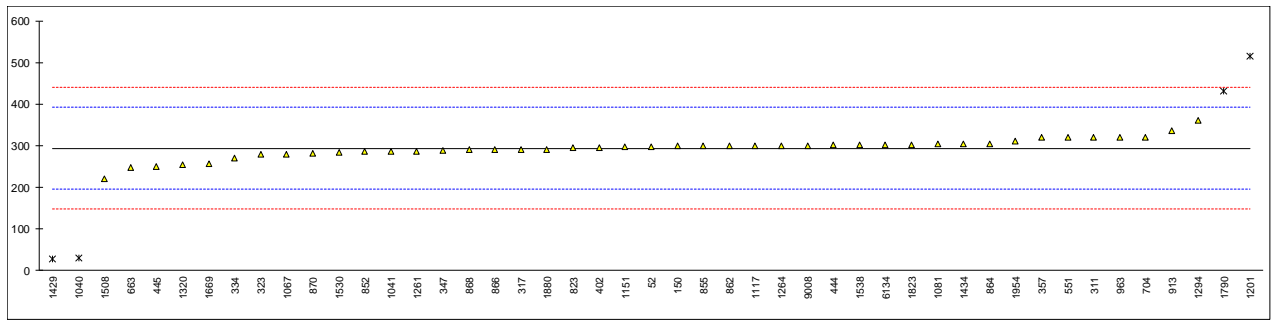
Determination of Nonaromatics on sample #18020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7504	81		0.78	
150	D4492	80	C	0.69	first reported: 0.008
174		-----		-----	
311	D4492	70		-0.20	
317	D4492	45	C	-2.42	first reported: 110
323	D7504	71		-0.11	
334	D4492	50	C	-1.98	first reported: 0.005
347	D4492	72		-0.02	
357	D4492	55		-1.53	
402	D4492	105.05		2.91	
444	D4492	82		0.87	
445	D4492	34		-3.40	
551	D4492	78		0.51	
555		-----		-----	
663	D4492	78.2		0.53	
704	D4492	88		1.40	
823	D7360	78		0.51	
852	D4492	74		0.16	
855	D4492	70		-0.20	
862	D4492	81		0.78	
864	D4492	66		-0.55	
866	D4492	81		0.78	
868	D4492	82		0.87	
870	D4492	83		0.96	
912		-----		-----	
913	D4492	35		-3.31	
962		-----		-----	
963	D4492	50		-1.98	
1040	D7504	74.0		0.16	
1041	In house	89		1.49	
1067	In house	60		-1.09	
1081	D4492	86.737		1.29	
1117	D4492	80		0.69	
1151		-----		-----	
1201	D4492	80		0.69	
1261	D4492	83		0.96	
1264	D4492	79		0.60	
1294	D4492	210	C,R(0.01)	12.24	first reported: 0.021
1320	D4492	29.85		-3.76	
1429	D4492	70		-0.20	
1434	D4492	61.2		-0.98	
1508	D2360	138	C,R(0.01)	5.84	first reported: 2043
1530	D4492	52		-1.80	
1538	D7504	76		0.33	
1669	D5713	66		-0.55	
1790	D4492	84		1.04	
1823	D4492	85		1.13	
1880	D4492	76		0.33	
1954	D4492	83.8		1.03	
6134	D4492	87.73		1.38	
9008	D4492	86		1.22	

|			
	normality	OK	
	n	44	
	outliers	2	
	mean (n)	72.24	
	st.dev. (n)	16.099	
	R(calc.)	45.08	
	st.dev.(D4492:10)	11.259	
	R(D4492:10)	31.53	

Kernel Density
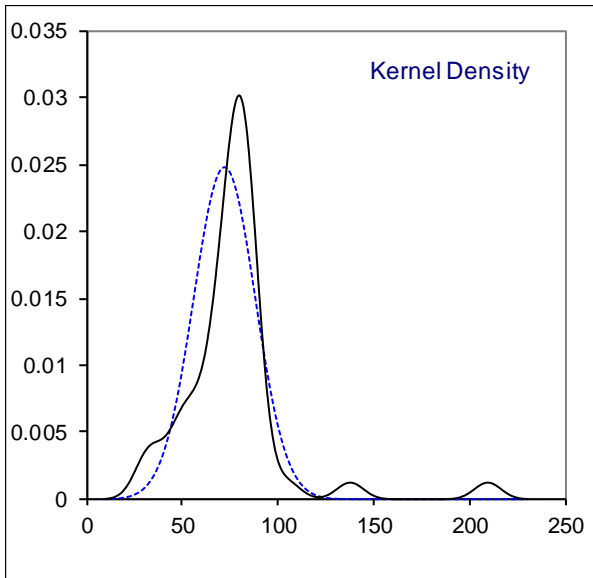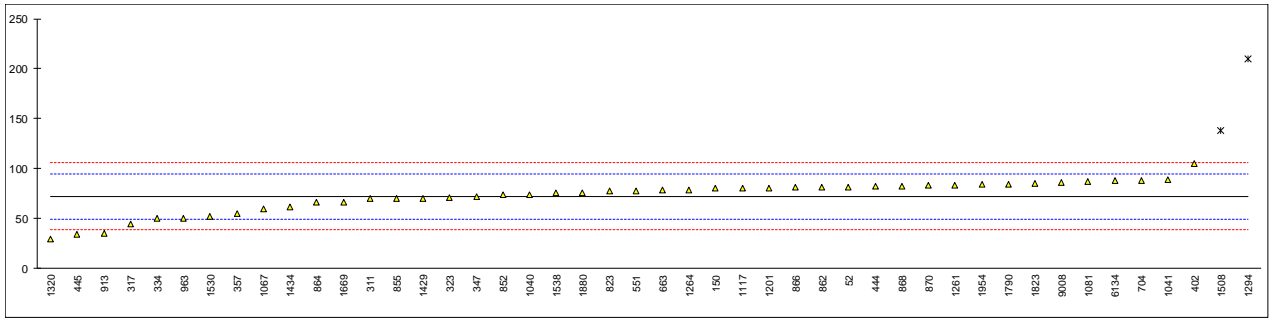
Determination of 1,4-Dioxane on sample #18020; results in mg/kg

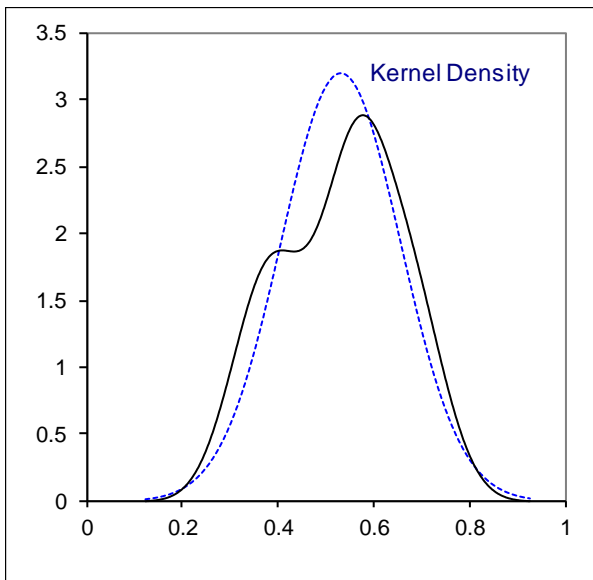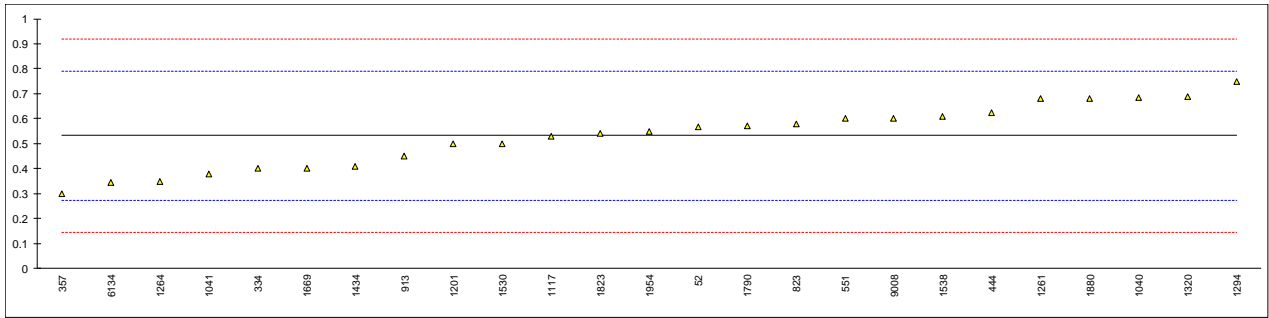| lab	method	value	mark	z(targ)	remarks
52	D7504	<1		-----	
150		-----		-----	
174		-----		-----	
311		-----		-----	
317		-----		-----	
323		-----		-----	
334		-----		-----	
347		-----		-----	
357	D4492	< 5		-----	
402	D4492	0		-----	
444		-----		-----	
445	D4492	<5		-----	
551	D4492	<5		-----	
555	D4492	<5		-----	
663	UOP921	<1		-----	
704	D4492	<5		-----	
823	D7360	<10		-----	
852	D4492	<5		-----	
855	D4492	<10		-----	
862	D4492	<5		-----	
864	D4492	<10		-----	
866	D4492	0.9		-----	
868	D4492	<5		-----	
870	D4492	<10		-----	
912		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1040		-----		-----	
1041		-----		-----	
1067		-----		-----	
1081		-----		-----	
1117		-----		-----	
1151		-----		-----	
1201		-----		-----	
1261		-----		-----	
1264	D4492	Not Detected		-----	
1294	D4492	0.000		-----	
1320	D4492	<5		-----	
1429		-----		-----	
1434	D4492	0.0000		-----	
1508		-----		-----	
1530		-----		-----	
1538		-----		-----	
1669	D4492	<5		-----	
1790		-----		-----	
1823		-----		-----	
1880		-----		-----	
1954	D4492	0.54		-----	
6134		-----		-----	
9008		-----		-----	
	n	22			
	mean (n)	<10			

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Determination of Solidification Point (anhydrous basis) on sample #18020; results in °C

lab	method	value	mark	z(targ)	remarks
52	D852	5.47		-0.71	
150	D852	5.50		0.97	
174		-----		-----	
311	D852	5.51		1.53	
317		-----		-----	
323	D852	5.48		-0.15	
334		-----		-----	
347		-----		-----	
357	D852	5.51		1.53	
402		-----		-----	
444		-----		-----	
445		-----		-----	
551	D852	5.48		-0.15	
555	D852	5.49		0.41	
663		-----		-----	
704		-----		-----	
823		-----		-----	
852	D852	5.48		-0.15	
855	D852	5.48		-0.15	
862	D852	5.48		-0.15	
864	D852	5.48		-0.15	
866	D852	5.47		-0.71	
868	D852	5.47		-0.71	
870	D852	5.47		-0.71	
912		-----		-----	
913	D852	5.49		0.41	
962		-----		-----	
963	D852	5.49		0.41	
1040	DIN51798	5.49		0.41	
1041		-----		-----	
1067	D852	5.45		-1.83	
1081		-----		-----	
1117		-----		-----	
1151		-----		-----	
1201		-----		-----	
1261	D852	5.48		-0.15	
1264	D852	5.47		-0.71	
1294	D852	5.4	R(0.01)	-4.63	
1320		-----		-----	
1429	D852	5.496		0.75	
1434		-----		-----	
1508		-----		-----	
1530		-----		-----	
1538	D852	5.48		-0.15	
1669		-----		-----	
1790		-----		-----	
1823		-----		-----	
1880	D852	5.49		0.41	
1954	D852	5.47		-0.71	
6134	D852	5.49		0.41	
9008		-----		-----	
	normality	OK			
	n	25			
	outliers	1			
	mean (n)	5.483			
	st.dev. (n)	0.0135			
	R(calc.)	0.038			
	st.dev.(D852:16)	0.0179			
	R(D852:16)	0.05			

Kernel Density
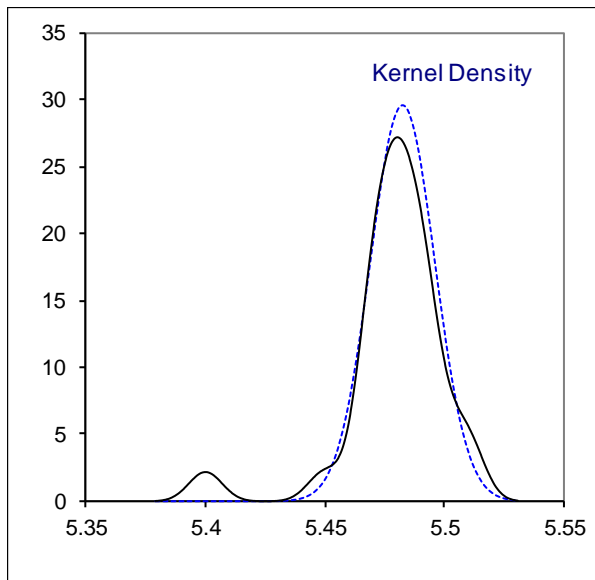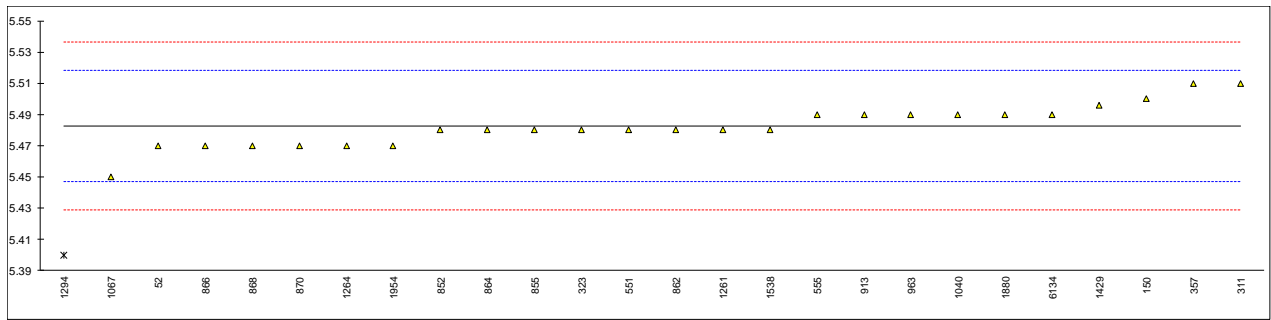
Determination of Sulphur on sample #18020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7183	0.568		0.28	
150		-----		-----	
174	D5453	<1		-----	
311	D5453	<1.0		-----	
317	D5453	<1.0		-----	
323	D5453	< 1.0		-----	
334	ISO20846	0.4		-1.02	
347	D5453	<1		-----	
357	D7183	0.3		-1.80	
402	D5453	<1		-----	
444	D5453	0.624		0.72	
445	D5453	<1		-----	
551	D5453	0.6		0.53	
555	D7039	<3.2		-----	
663		-----		-----	
704	D5453	<1		-----	
823	D7183	0.58		0.38	
852	SH/T0253	<1		-----	
855	D7183	<1		-----	
862		-----		-----	
864	D7183	<1		-----	
866		-----		-----	
868	D5453	<1		-----	
870		-----		-----	
912	D5453	<1		-----	
913	D5453	0.45		-0.63	
962		-----		-----	
963		-----		-----	
1040	ISO20846	0.685		1.19	
1041	D5453	0.38		-1.18	
1067	D5453	< 1.0		-----	
1081		-----		-----	
1117	D5453	0.53		-0.01	
1151		-----		-----	
1201	D5453	0.5		-0.24	
1261	D7183	0.68		1.15	
1264	D5453	0.35		-1.41	
1294	D4045	0.75		1.69	
1320	ISO20846	0.69		1.23	
1429	D5453	< 0.5		-----	
1434	D7183	0.4084		-0.96	
1508		-----	W	-----	first reported: 25 (D5623, D4735 & D4045)
1530	D5453	0.5		-0.24	
1538	D7183	0.61		0.61	
1669	D5453	0.4		-1.02	
1790	D5453	0.57		0.30	
1823	D5453	0.54		0.07	
1880	D5453	0.68		1.15	
1954	D7183	0.55		0.14	
6134	D5453	0.3436		-1.46	
9008	D5453	0.6		0.53	

	normality	OK	
	n	25	
	outliers	0	
	mean (n)	0.5316	
	st.dev. (n)	0.12473	
	R(calc.)	0.3492	
	st.dev.(D5453:16e1)	0.12889	
	R(D5453:16e1)	0.3609	

Kernel Density

Determination of Thiophene on Benzene sample #18020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D4735	0.211		-----	
150		-----		-----	
174		-----		-----	
311		-----		-----	
317		-----		-----	
323		-----		-----	
334		-----		-----	
347		-----		-----	
357		-----		-----	
402		-----		-----	
444		-----		-----	
445		-----		-----	
551		-----		-----	
555		-----		-----	
663		-----		-----	
704		-----		-----	
823	D4735	<0.80		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		0.25		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1040		-----		-----	
1041		-----		-----	
1067		-----		-----	
1081		-----		-----	
1117		-----		-----	
1151		-----		-----	
1201	In house	0.34		-----	
1261		-----		-----	
1264	D7011	0.25		-----	
1294	D4735	<1		-----	
1320		-----		-----	
1429		-----		-----	
1434		-----		-----	
1508	D5623	0.08	C	-----	first reported: 0.8
1530		-----		-----	
1538		-----		-----	
1669		-----		-----	
1790	D7011	0.097		-----	
1823		-----		-----	
1880	D4735	0.096		-----	
1954		-----		-----	
6134	D7011	0.1398		-----	
9008		-----		-----	

normality	unknown
n	8
outliers	0
mean (n)	0.1830
st.dev. (n)	0.09400
R(calc.)	0.2632
st.dev.(D7011:15)	(0.052343)
R(D7011:15)	(0.1466)

APPENDIX 2

Number of participants

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

APPENDIX 3

Abbreviations:

C   = final test result after checking of first reported suspect test result
D(0.01)   = outlier in Dixon's outlier test
D(0.05)   = straggler in Dixon's outlier test
G(0.01)   = outlier in Grubbs' outlier test
G(0.05)   = straggler in Grubbs' outlier test
DG(0.01)   = outlier in Double Grubbs' outlier test
DG(0.05)   = straggler in Double Grubbs' outlier test
R(0.01)   = outlier in Rosner's outlier test
R(0.05)   = straggler in Rosner's outlier test
E   = probably an error in calculations
U   = test result probably reported in a different unit
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

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