Results of Proficiency Test
Styrene
October 2018

Organised by: Institute for Interlaboratory Studies
Spijkenisse, the Netherlands

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CONTENTS

1 INTRODUCTION

Since 1995, the Institute for Interlaboratory Studies (iis) organizes a proficiency test for the analyses of Styrene. During the annual proficiency testing program 2018/2019, it was decided to continue the round robin for the analyses of Styrene in accordance with the latest applicable version of the product specification ASTM D2827.
In this interlaboratory study, 41 laboratories from 20 different countries registered for participation. See appendix 2 for the number of participants per country.
In this report, the results of the 2018 Styrene 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 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/IEC 17025 accredited laboratory. It was decided to send one 0.5 litre bottle with Styrene monomer.
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% confidentially 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 SAMPLES

The necessary bulk material of Styrene was obtained from a local Styrene producer. To 32 kg of this batch 98.6 mg Chloroform was added.
After homogenisation, 64 amber glass bottles of 0.5 L were filled and labelled #18190. The homogeneity of subsamples #18190 was checked by determination of Density at 20°C in accordance with ASTM D4052 and Chloride (Organic) in accordance with ASTM D5808 on stratified randomly selected samples.

	Density at 20°C in kg/L	*Chloride (Organic) in mg Cl/kg*
sample #18190-1	0.90624	1.80
sample #18190-2	0.90624	2.29
sample #18190-3	0.90624	2.04
sample #18190-4	0.90624	2.40
sample #18190-5	0.90625	1.96
sample #18190-6	0.90624	1.62
sample #18190-7	0.90624	2.17
sample #18190-8	0.90625	2.11

Table1: homogeneity test results of subsamples #18190

From the above test results, the repeatabilities were calculated and compared with 0.3 times the corresponding reproducibility or with the repeatability 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	*Chloride (Organic) in mg Cl/kg*
r (observed)	0.00001	0.71
ref. test method	ISO 12185:96	ASTM D5808:18
0.3 x R (ref. test method)	0.00015	--
r (ref. test method)	--	0.7

Table 2: evaluation of the repeatabilities of subsamples #18190

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

To each of the participating laboratories, 1 bottle of 0.5 L (labelled #18190) was sent on September 19, 2018. An SDS was added to the sample package.

2.5 STABILITY OF THE SAMPLES

The stability of Styrene 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 #18190: Aldehydes as Benzaldehyde, Appearance, Chloride (Organic), Color Pt/Co, Density at 20°C, Inhibitor as TBC, Peroxide as H_2O_2, Polymer, Sulphur, Water (coulometric KF titration), Purity and the Impurities by GC; Benzene, Toluene, Ethylbenzene, m- + p- Xylene, iso-Propylbenzene (Cumene), o-Xylene, n-Propylbenzene, m- + p-Ethyltoluene, α-Methylstyrene, 1,2-Diethylbenzene, sum α-Methylstyrene and 1,2-Diethylbenzene, Phenylacetylene, 3/4-Methylstyrenes, sum Phenylacetylene and 3/4-Dimethylstyrenes, Benzaldehyde and Nonaromatics. It was requested to report some analytical details on the determination of Aldehydes as Benzaldehyde.

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

3.1 STATISTICS

The protocol followed in the organization of this proficiency test was the one as described for proficiency testing in the report 'iis Interlaboratory Studies: Protocol for the Organisation, Statistics and Evaluation' of June 2018 (iis-protocol, version 3.5).

For the statistical evaluation the *unrounded* (when available) figures were used instead of the rounded test results. Test results reported as '<…' or '>…' were not used in the statistical evaluation.
First, the normality of the distribution of the various data sets per determination was checked by means of the Lilliefors-test, a variant of the Kolmogorov-Smirnov test and by the calculation of skewness and kurtosis. Evaluation of the three normality indicators in combination with the visual evaluation of the graphic Kernel density plot, lead to judgement of the normality being either 'unknown', 'OK', 'suspect' or 'not OK'. After removal of outliers, this check was repeated. If a data set does not have a normal distribution, the results of the statistical evaluation should be used with due care.

According to ISO 5725 the original test results per determination were submitted to Dixon's, 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 visualise 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 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.

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. 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 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. Ten participants reported after the final reporting date and two participants did not report any test results at all.
Not all participants were able to report all requested parameters. Finally, 39 laboratories did report 649 numerical test results. Observed were 25 outlying test results, which is 3.9%. 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 test 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. D2119) and an added designation for the year that the test method was adopted or revised (e.g. D2119:09). If applicable, a designation in parentheses is added to designate the year of withdrawn (e.g. D2119:09(withdrawn 2018)).

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 reproducibility estimated from the Horwitz equation.

Aldehydes as Benzaldehyde: This determination was problematic. Two statistical outliers were observed and eight other test results were excluded. Test method ASTM D2119 describes the use of 0.05N NaOH. Therefore, test results of ASTM D2119 and reported to use 0.01N or 0.02N NaOH were excluded from the statistical evaluation. Test results were also excluded when the reported Aldehyde as Benzaldehyde results were less than the test result for Benzaldehyde by GC. The calculated reproducibility after rejection of the suspect data is not in agreement with the requirements of ASTM D2119:09(withdrawn 2018).
Two laboratories reported to have used ASTM D7704 as test method. ASTM D7704 describes the use of 0.02N NaOH.

Appearance: Allthough not mentioned the specification of Styrene (ASTM D2827:13), it is advised to use test method ASTM E2680:09(2015)e1 for the appearance determination. All participants agreed about the appearance of sample #18190 to be ‘clear’, ‘bright’ or ‘pass’. Participants who used ASTM E2680 should report the appearance as ‘pass’ or as ‘fail’ as test result.

Chloride, Organic: 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 D5808:18. The average recovery of Organic Chloride (theoretical increment of 2.31 mg Cl/kg) may be good: “less than 114%” (the actual blank Chloride content is not known).

Color Pt/Co: 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 D5386:16 and with ASTM D1209:05(2011).

Density at 20°C: 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 ISO 12185:96.

Inhibitor as TBC: This determination was not problematic. No statisticals outliers were observed. The calculated reproducibility is in full agreement with the requirements of ASTM D4590:18.

Peroxides as H_2O_2: This determination was problematic. No statistical outliers were observed. However, the calculated reproducibility is not in agreement with the requirements of ASTM D2340:18.

Polymer: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D2121-A:16.

Sulphur: This determination was not problematic. One statistical outlier was observed. However, the calculated reproducibility after rejection of the statistical outlier is in full agreement with the requirements of ASTM D5453:16e1.

Water, coulometric KF titration: 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 requirement of ASTM E1064:16.

Purity by GC: This determination was problematic. No statistical outliers were observed. However, the calculated reproducibility is not in agreement with the requirements of ASTM D5135:16e1.

Benzene: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D5135:16e1.

Toluene: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in full agreement with the estimated reproducibility using the Horwitz equation.

Ethylbenzene: 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 ASTM D5135:16e1.

m- + p-Xylene: 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 D5135:16e1.

iso-Propylbenzene: This determination was problematic. Two statistical outliers were observed. The calculated reproducibility after rejection of the statistical outliers is not in agreement with the requirements of ASTM D5135:16e1.

o-Xylene: 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 D5135:16e1.

n-Propylbenzene: This determination was problematic. One statistical outlier was observed. The calculated reproducibility after rejection of the statistical outlier is not in agreement with the requirements of ASTM D5135:16e1.

m- + p-Ethyltoluene: 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 D5135:16e1.

α-Methylstyrene: This determination was problematic. No statistical outliers were observed. However, the calculated reproducibility is not in agreement with the requirements of ASTM D5135:16e1.

1,2-Diethylbenzene: Three laboratories reported a numeric test result and one laboratory reported a test value “<10”. Therefore, no z-scores were calculated.

Sum α-Methylstyrene & 1,2-Diethylbenzene: Only five laboratories reported a numerical test result for the sum of the two components. No statistical outliers were observed. The level of the sum of the two components is close to the level of α-Methylstyrene as the level of 1,2-Diethylbenzene is below the detection limit. No z-scores were calculated

Phenylacetylene: This determination was not problematic. One statistical outlier was observed and two other test results were excluded from the statistical evaluation as the summation of the test results of Phenylacetylene and the test result of 3/4-Methylstyrenes is not in line with the reported test result of 'sum of Phenylacetylene and 3/4-Methylstyrenes'. However, the calculated reproducibility after rejection of the suspect data is in full agreement with the requirements of ASTM D5135:16e1.

3/4-Methylstyrenes: This determination may not be problematic. No statistical outliers were observed, but two test results were excluded from the statistical evaluation as the summation of the test results of Phenylacetylene and the test result of 3/4-Methylstyrenes is not in line with the reported test result of 'sum of Phenylacetylene and 3/4-Methylstyrenes'. The calculated reproducibility after rejection of the suspect data is in full agreement with the estimated target reproducibility using the Horwitz equation for 2 components.

Sum Phenylacetylene & 3/4-Methylstyrenes: This determination may be problematic. No statistical outliers were observed, but two test results were excluded from the statistical evaluation as the summation of the test results of Phenylacetylene and the test result of 3/4-Methylstyrenes is not in line with the reported test result of 'sum of Phenylacetylene and 3/4-Methylstyrenes'. However, the calculated reproducibility was not at all in agreement with the estimated target reproducibility using the Horwitz equation for 3 components. Therefore, it was decided not to calculate z-scores.

Benzaldehyde: This determination was very problematic. No statistical outliers were observed, but two test results were excluded from the statistical evaluation as the reported test results for Benzaldehyde by GC were higher than the reported Aldehyde as Benzaldehyde results. The calculated reproducibility after rejection of the suspect data is not at all in agreement with the requirements of ASTM D5135:16e1.

Nonaromatics: This determination was not problematic. Three statistical outliers were observed. However, the calculated reproducibility after rejection of the statistical outliers is in full agreement with the requirements of ASTM D5135:16e1.

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 result, the calculated reproducibility (2.8 * standard deviation) and the target reproducibilities derived from reference test methods (in casu ASTM test methods).

Parameter	unit	n	average	2.8 * sd	R (lit)
Aldehydes as Benzaldehyde	mg/kg	17	83.0	60.8	33.2
Appearance		36	Pass	n.a.	n.a.
Chloride, Organic	mg/kg	15	2.6	1.1	1.3
Color Pt/Co		36	8.1	3.8	5.9
Density at 20°C	kg/L	32	0.9063	0.0002	0.0005
Inhibitor as TBC	mg/kg	37	8.5	3.3	3.0
Peroxides as H_2O_2	mg/kg	31	23.9	19.0	13
Polymer	mg/kg	31	1.1	0.9	3.2
Sulphur	mg/kg	18	0.53	0.39	0.36
Water, coulometric KF titration	mg/kg	36	162	28	45
Purity by GC	%M/M	34	99.91	0.04	0.02
Benzene	mg/kg	28	8.4	2.5	3.6
Toluene	mg/kg	24	77.8	19.6	18.1
Ethylbenzene	mg/kg	31	201	30	47
m- + p-Xylene	mg/kg	28	57.1	8.8	10.9
iso-Propylbenzene (Cumene)	mg/kg	29	43.2	9.1	7.0
o-Xylene	mg/kg	27	30.1	4.9	7.5
n-Propylbenzene	mg/kg	28	73.8	24.2	18.5
m- + p-Ethyltoluene	mg/kg	21	27.4	8.5	10.9
α-Methylstyrene	mg/kg	31	265	58	41
1,2-Diethylbenzene	mg/kg	4	<10	n.a.	n.a.
sum α-Methylstyrene & 1,2-Diethylbenzene	mg/kg	5	267	101	(41)
Phenylacetylene	mg/kg	25	19.4	18.2	19.4
3/4-Methylstyrenes	mg/kg	4	8.7	4.0	4.0
sum Phenylacetylene & 3/4-Methylstyrenes	mg/kg	6	21.5	19.1	(10.5)
Benzaldehyde	mg/kg	17	49.6	37.7	18.6
Nonaromatics	mg/kg	14	33.7	40.6	39.3

Table 3: reproducibilities of tests on sample #18190

Between brackets is should be used with due care

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

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

	October 2018	*October 2017*	*October 2016*	*October 2015*	*September 2014*
Number of reporting labs	39	38	38	37	36
Number of test results reported	649	524	521	447	510
Number of statistical outliers	25	24	14	20	33
Percentage outliers	3.9%	4.6%	2.7%	4.5%	6.5%

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 in the following table:

Parameter	*October 2018*	*October 2017*	*October 2016*	*October 2015*	*September 2014*
Aldehydes as Benzaldehyde	--	-	-	--	--
Chloride, Organic	+	+	+	n.e.	+
Color Pt/Co	+	++	+	++	++
Density at 20°C	++	++	++	++	++
Inhibitor as TBC	+/-	+	+/-	+	--
Peroxides as H_2O_2	-	-	-	-	--
Polymer	++	+	-	++	--
Sulphur	+/-	+/-	+	n.e.	+
Water, coulometric KF titration	+	++	+	+	++
Purity by GC	--	+	+/-	+	(--)
Benzene	+	++	-	n.e.	--
Toluene	+/-	n.e.	n.e.	n.e.	--
Ethylbenzene	+	++	+	++	++
m- + p-Xylene	+	n.e.	n.e.	++	++
iso-Propylbenzene (Cumene)	-	n.e.	n.e.	-	--
o-Xylene	+	+	n.e.	++	--
n-Propylbenzene	-	n.e.	+	(--)	--
m- + p-Ethyltoluene	+	n.e.	+	(-)	++
α-Methylstyrene	-	+	--	++	--
1,2-Diethylbenzene	n.e.	n.e.	(--)	n.e.	(--)
sum α-Methylstyrene & 1,2-Diethylbenzene	(--)	+/-	+/-	++	n.e.
Phenylacetylene	+/-	n.e.	n.e.	n.e.	--
3/4-Methylstyrenes	+/-	n.e.	n.e.	n.e.	n.e.
sum Phenylacetylene & 3/4-Methylstyrenes	(--)	n.e.	+	n.e.	n.e.
Benzaldehyde	--	+	-	-	--
Nonaromatics	+/-	+	--	n.e.	--

Table 5: comparison of overall performance against the requirements of the reference test method per parameter

Between brackets is should be used with due care

The following performance categories were used:

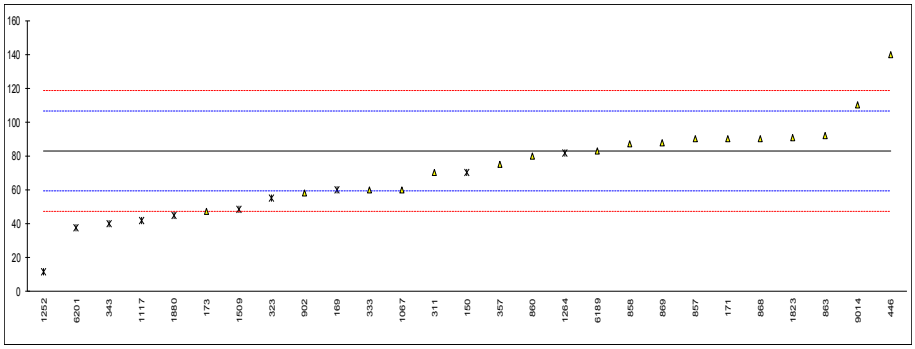
++ : group performed much better than the reference test method
+ : group performed better than the reference test method
+/- : group performance equals the reference test method
- : group performed worse than the reference test method
-- : group performed much worse than the reference test method
n.e.: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

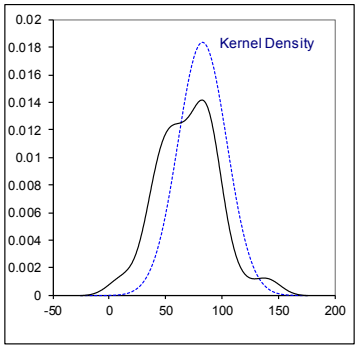
APPENDIX 1

Determination of Aldehydes as Benzaldehyde on sample #18190; results in mg/kg

lab	method	N NaOH	value	mark	z(targ)	remarks
131		-----	-----		-----	
150	D2119	0.01	70	ex	-1.10	excluded, see § 4.1
169	D2119	0.02	60	ex	-1.94	excluded, see § 4.1
171	D2119	0.05	90		0.59	
173	D2119	0.05	47		-3.04	
273		-----	-----		-----	
311	D2119	0.05	70		-1.10	
323	D2119	0.05	55	ex	-2.36	excluded, see § 4.1
333	D2119	0.05	60		-1.94	
343	D2119	-----	40	ex	-3.63	excluded, see § 4.1
347		-----	-----		-----	
357	D2119	0.05	75		-0.67	
446	D2119	0.05	140		4.81	
551		-----	-----		-----	
613		-----	-----		-----	
857	D2119	0.05	90		0.59	
858	D2119	0.05	87		0.34	
860	D2119	0.05	80		-0.25	
863	D2119	0.05	92		0.76	
868	D2119	0.05	90		0.59	
869	D2119	0.05	88		0.42	
902	D2119	0.05	58		-2.11	
913		-----	-----		-----	
1067	D2119	0.05	60		-1.94	
1117	D7704	0.02	42.030	G(0.05)	-3.46	
1135		-----	-----		-----	
1169		-----	-----		-----	
1201		-----	-----		-----	
1252	D2119	0.01	11.4	ex	-6.04	excluded, see § 4.1
1264	D2119	0.01	82	ex	-0.08	excluded, see § 4.1
1509	D2119	0.01	48.6	ex	-2.90	excluded, see § 4.1
1515		-----	-----		-----	
1823	D2119	0.05	91		0.67	
1880	D7704	0.02	45	G(0.05)	-3.20	
1935		-----	-----		-----	
6189	D2119	0.05	83	C	0.00	reported 0.0083 mg/kg (unit error?)
6201	D2119	0.02	37.6	ex,C	-3.83	first reported 0.00376 mg/kg, excluded, see § 4.1
6202		-----	-----		-----	
7014		-----	-----		-----	
9008		-----	-----		-----	
9014	D2119	0.0508	110		2.28	

normality	not OK	
n	17	
outliers	2 (+8 ex)	
mean (n)	83.00	
st.dev. (n)	21.697	
R(calc.)	60.75	
st.dev.(D2119:09)	11.857	
R(D2119:09(withdrawn))	33.20	Compare R(D7704:16) = 106





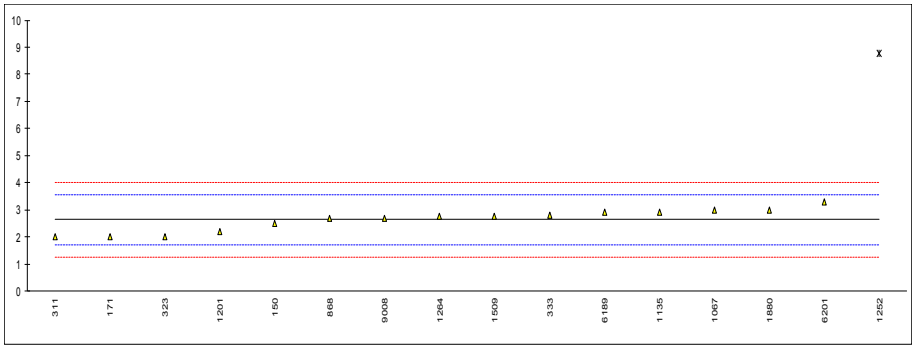
Determination of Appearance on sample #18190;

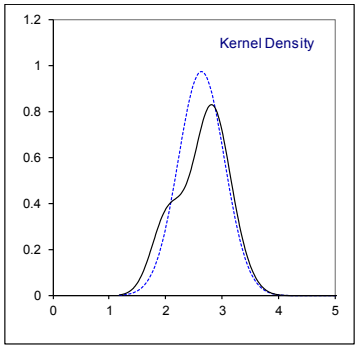
lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D4176	C&B		-----	
169	Visual	C&FSM		-----	
171	E2680	Pass		-----	
173	D4176	Pass		-----	
273	Visual	B&C		-----	
311	E2680	pass		-----	
323	D4176	pass		-----	
333		-----		-----	
343	E2680	pass		-----	
347	E2680	Pass		-----	
357	E2680	Pass		-----	
446	E2680	Pass		-----	
551	E2680	PASS		-----	
613	E2680	Clear&Clean		-----	
857	E2680	Pass		-----	
858	E2680	PASS		-----	
860	E2680	Pass		-----	
863	Visual	Pass		-----	
868	E2680	PASS		-----	
869	Visual	Clear and free from suspended matter.		-----	
902	E2680	PASS		-----	
913		-----		-----	
1067	Visual	Bright and Clear		-----	
1117	D4176	PASS		-----	
1135	D4176	pass		-----	
1169	Visual	Bright, 2 particulates		-----	
1201	D4176	Br & Cl		-----	
1252	Visual	PASS		-----	
1264	Visual	pass		-----	
1509	E2680	Clear & FFSM		-----	
1515	E2680	Pass		-----	
1823	D4176	Clear and free suspended water		-----	
1880	Visual	Pass		-----	
1935		-----		-----	
6189	E2680	Pass		-----	
6201	D4176	Bright and Clear		-----	
6202		-----		-----	
7014	Visual	Clear		-----	
9008	Visual	Clear liquid		-----	
9014	E2680	pass		-----	
	n	36			
	mean (n)	Pass			

Determination of Chloride, Organic on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D7359	2.5		-0.29	
169		-----		-----	
171	D5808	2		-1.37	
173		-----		-----	
273		-----		-----	
311	D5808	2		-1.37	
323	D5808	2		-1.37	
333	D5808	2.8		0.35	
343		-----		-----	
347		-----		-----	
357		-----		-----	
446		-----		-----	
551		-----		-----	
613		-----		-----	
857		-----		-----	
858		-----		-----	
860		-----		-----	
863		-----		-----	
868	D5808	2.7		0.14	
869		-----		-----	
902		-----		-----	
913		-----		-----	
1067	D5808	3		0.78	
1117		-----		-----	
1135	D5808	2.93		0.63	
1169		-----		-----	
1201	D5808	2.2		-0.94	
1252	UOP395	8.79	G(0.01)	13.25	
1264	D5808	2.75		0.25	
1509	D5808	2.76		0.27	
1515		-----		-----	
1823		-----		-----	
1880	D7359	3.0		0.78	
1935		-----		-----	
6189	D5808	2.9		0.57	
6201	UOP779	3.3		1.43	
6202		-----		-----	
7014		-----		-----	
9008	D5808	2.7		0.14	
9014		-----		-----	

normality	OK	
n	15	
outliers	1	spike
mean (n)	2.636	2.31 (recovery: <114%)
st.dev. (n)	0.4095	
R(calc.)	1.147	
st.dev.(D5808:18)	0.4643	
R(D5808:18)	1.3	



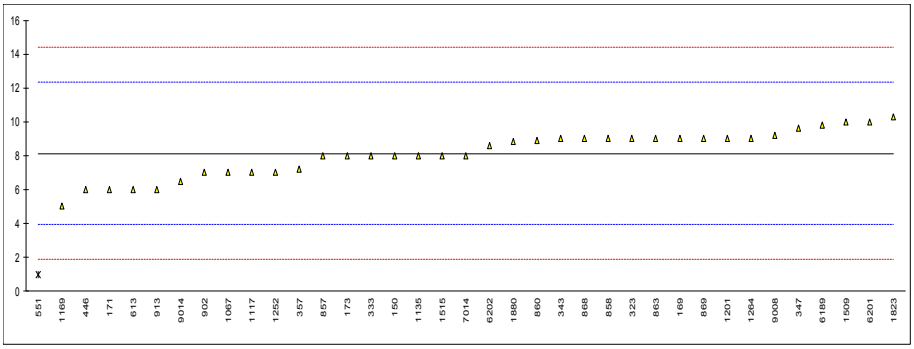


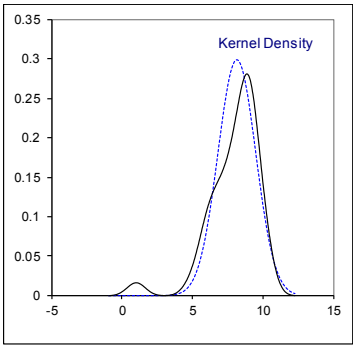
Determination of Color Pt/Co on sample #18190;

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5386	8		-0.07	
169	D5386	9.0		0.41	
171	D5386	6		-1.02	
173	D5386	8		-0.07	
273	D1209	<5		-----	
311		-----		-----	
323	D5386	9		0.41	
333	D5386	8		-0.07	
343	D5386	9		0.41	
347	D5386	9.6		0.70	
357	D5386	7.2		-0.45	
446	D5386	6		-1.02	
551	D5386	1	R(0.01)	-3.41	
613	D5386	6		-1.02	
857	D5386	8		-0.07	
858	D5386	9		0.41	
860	D5386	8.9		0.36	
863	D1209	9		0.41	
868	D5386	9.0		0.41	
869	D1209	9		0.41	
902	D5386	7		-0.54	
913	D5386	6		-1.02	
1067	D5386	7		-0.54	
1117	D1209	7		-0.54	
1135	D5386	8		-0.07	
1169	D1209	5	C	-1.50	first reported 17
1201	D5386	9		0.41	
1252	D1209	7		-0.54	
1264	D1209	9		0.41	
1509	D1209	10		0.89	
1515	D1209	8		-0.07	
1823	D5386	10.3		1.03	
1880	D5386	8.85		0.34	
1935		-----		-----	
6189	D5386	9.8		0.79	
6201	D5386	10		0.89	
6202	D1209	8.59		0.22	
7014	D1209	8		-0.07	
9008	D5386	9.2		0.51	
9014	D5386	6.5		-0.78	

normality	OK
n	36
outliers	1
mean (n)	8.14
st.dev. (n)	1.338
R(calc.)	3.75
st.dev.(D5386:16)	2.092
R(D5386:16)	5.86

Compare R(D1209:05(2011)) = 7

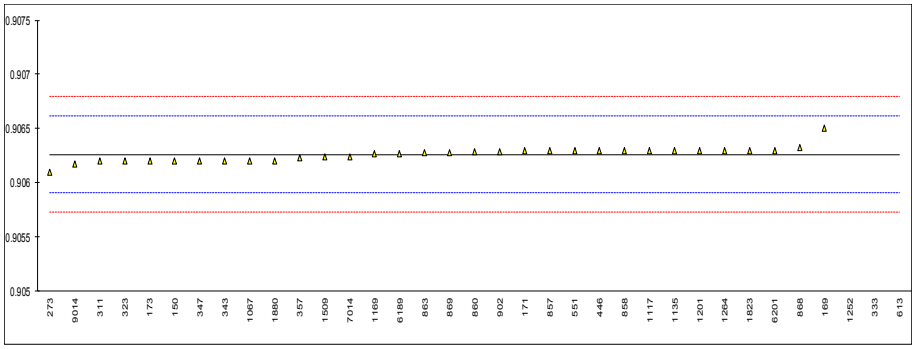


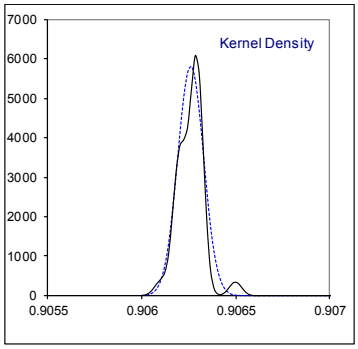


Determination of Density at 20°C on sample #18190; results in kg/L

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D4052	0.9062		-0.35	
169	D4052	0.9065		1.33	
171	D4052	0.9063		0.21	
173	D4052	0.9062		-0.35	
273	D4052	0.9061		-0.91	
311	D4052	0.9062		-0.35	
323	ISO12185	0.9062		-0.35	
333	ISO12185	0.9106	R(0.01)	24.29	
343	D4052	0.9062		-0.35	
347	D4052	0.9062		-0.35	
357	D4052	0.90623		-0.18	
446	D4052	0.9063		0.21	
551	D4052	0.9063		0.21	
613	D4052	0.9111	R(0.01)	27.09	measured at 15 °C
857	D4052	0.90630		0.21	
858	D4052	0.90630		0.21	
860	D4052	0.90629		0.16	
863	D4052	0.90628		0.10	
868	D4052	0.90632		0.33	
869	D4052	0.90628		0.10	
902	D4052	0.90629		0.16	
913		-----		-----	
1067	ISO12185	0.9062		-0.35	
1117	D4052	0.9063		0.21	
1135	ISO12185	0.9063		0.21	
1169	D4052	0.90627		0.05	
1201	D4052	0.9063		0.21	
1252	D4052	0.9105	R(0.01)	23.73	
1264	D4052	0.9063		0.21	
1509	D4052	0.90624		-0.12	
1515		-----		-----	
1823	D4052	0.9063		0.21	
1880	D4052	0.9062		-0.35	
1935		-----		-----	
6189	D4052	0.90627		0.05	
6201	ISO12185	0.9063		0.21	
6202		-----		-----	
7014	D4052	0.90624		-0.12	
9008		-----		-----	
9014	D4052	0.90617		-0.51	

normality	not OK
n	32
outliers	3
mean (n)	0.90626
st.dev. (n)	0.000069
R(calc.)	0.00019
st.dev.(ISO12185:96)	0.000179
R(ISO12185:96)	0.0005

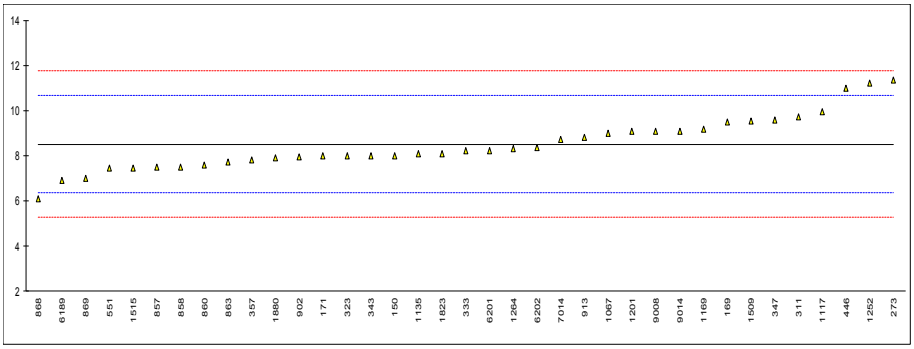


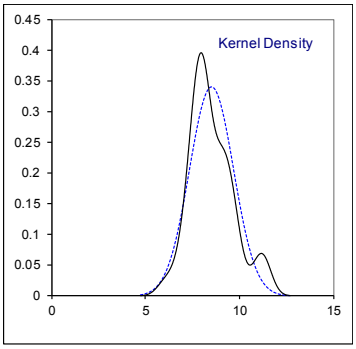


Determination of Inhibitor as TBC on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D4590	8		-0.48	
169	D4590	9.5		0.92	
171	D4590	8		-0.48	
173		-----		-----	
273	D4590	11.33		2.61	
311	D4590	9.7		1.10	
323	D4590	8	C	-0.48	first reported 4
333	D4590	8.2		-0.29	
343	D4590	8		-0.48	
347	D4590	9.6		1.01	
357	D4590	7.8		-0.66	
446	D4590	11		2.31	
551	D4590	7.45		-0.99	
613		-----		-----	
857	D4590	7.5		-0.94	
858	D4590	7.5		-0.94	
860	D4590	7.6		-0.85	
863	D4590	7.7		-0.75	
868	D4590	6.1		-2.24	
869	D4590	7.0		-1.40	
902	D4590	7.93		-0.54	
913	D4590	8.82		0.28	
1067	D4590	9		0.45	
1117	D4590	9.949		1.33	
1135	D4590	8.1		-0.38	
1169	D4590	9.19		0.63	
1201	D4590	9.1		0.54	
1252	D4590	11.2		2.49	
1264	D4590	8.3		-0.20	
1509	D4590	9.554		0.97	
1515	D4590	7.46080		-0.98	
1823	D4590	8.1		-0.38	
1880	D4590	7.9		-0.57	
1935		-----		-----	
6189	D4590	6.9		-1.50	
6201	D4590	8.2		-0.29	
6202	D4590	8.37		-0.13	
7014	D4590	8.72		0.19	
9008	In house	9.1		0.54	
9014	D4590	9.103		0.55	

normality	OK
n	37
outliers	0
mean (n)	8.513
st.dev. (n)	1.1702
R(calc.)	3.277
st.dev.(D4590:18)	1.0776
R(D4590:18)	3.017

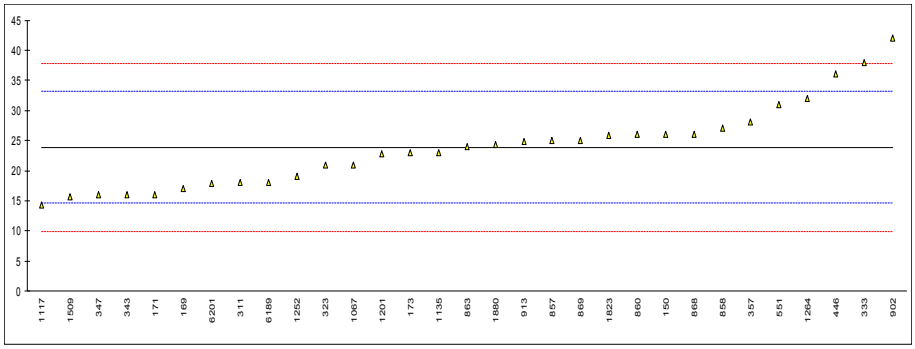


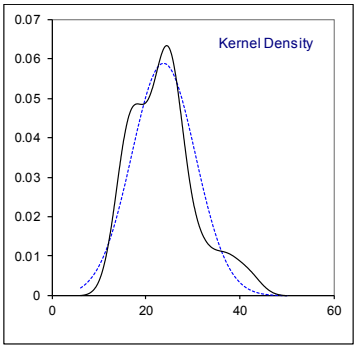


Determination of Peroxides as H_2O_2 on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D2340	26		0.46	
169	D2340	17		-1.48	
171	D2340	16		-1.69	
173	D2340	23		-0.19	
273		-----		-----	
311	D2340	18		-1.26	
323	D2340	21		-0.62	
333	D2340	38	C	3.04	first reported 57
343	D2340	16		-1.69	
347	D2340	16		-1.69	
357	D2340	28.0		0.89	
446	D2340	36		2.61	
551	D2340	31		1.54	
613		-----		-----	
857	D2340	25		0.24	
858	D2340	27		0.68	
860	D2340	26		0.46	
863	D2340	24		0.03	
868	D2340	26		0.46	
869	D2340	25		0.24	
902	D2340	42		3.91	
913	D2340	24.9	C	0.22	first reported 43.6
1067	D2340	21		-0.62	
1117	D2340	14.336		-2.05	
1135	D2340	23		-0.19	
1169		-----		-----	
1201	D2340	22.8		-0.23	
1252	D2340	19.1		-1.03	
1264	D2340	32		1.75	
1509	D2340	15.7		-1.76	
1515		-----		-----	
1823	D2340	25.8		0.42	
1880	D2340	24.3		0.09	
1935		-----		-----	
6189	D2340	18.0		-1.26	
6201	D2340	17.9		-1.28	
6202		-----		-----	
7014		-----		-----	
9008		-----		-----	
9014		-----		-----	

normality	OK
n	31
outliers	0
mean (n)	23.866
st.dev. (n)	6.7762
R(calc.)	18.973
st.dev.(D2340:18)	4.6429
R(D2340:18)	13

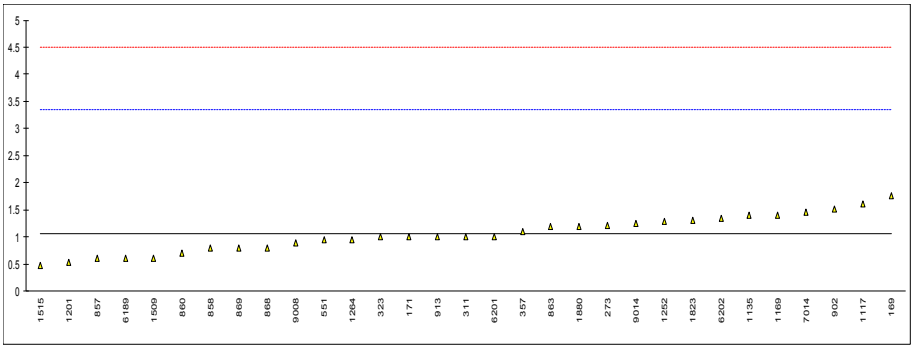


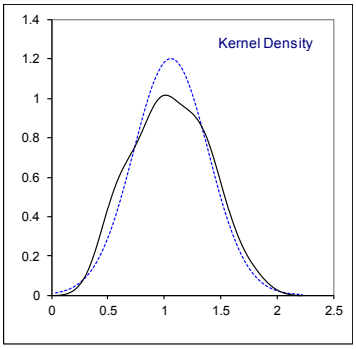


Determination of Polymer on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D2121-A	<1		-----	
169	D2121-A	1.769		0.62	
171	D2121-A	1		-0.05	
173		-----		-----	
273	D2121-A	1.22		0.14	
311	D2121-A	1		-0.05	
323	D2121-A	1		-0.05	
333		-----		-----	
343	D2121-A	<1		-----	
347	D2121-A	<1		-----	
357	D2121-A	1.1		0.04	
446	D2121-A	<1		-----	
551	D2121-A	0.95		-0.09	
613		-----		-----	
857	D2121-A	0.6		-0.40	
858	D2121-A	0.8		-0.22	
860	D2121-A	0.7		-0.31	
863	D2121-A	1.2		0.13	
868	D2121-A	0.8		-0.22	
869	D2121-A	0.8		-0.22	
902	D2121-A	1.51		0.40	
913	D2121-A	1.0		-0.05	
1067	D2121-A	< 1		-----	
1117	D2121-A	1.6		0.47	
1135	D2121-A	1.4		0.30	
1169	D2121-A	1.4		0.30	
1201	D2121-A	0.53		-0.46	
1252	D2121-A	1.28		0.19	
1264	D2121-A	0.95		-0.09	
1509	D2121-A	0.61		-0.39	
1515	D2121-A	0.48335		-0.50	
1823	D2121-A	1.3		0.21	
1880	D2121-A	1.2		0.13	
1935		-----		-----	
6189	D2121-A	0.6		-0.40	
6201	D2121-A	1.0		-0.05	
6202	D2121-A	1.354		0.26	
7014	D2121-A	1.45		0.34	
9008	D2121-A	0.9		-0.14	
9014	D2121-A	1.2465		0.17	

normality	OK
n	31
outliers	0
mean (n)	1.057
st.dev. (n)	0.3323
R(calc.)	0.930
st.dev.(D2121-A:16)	1.1461
R(D2121-A:16)	3.209



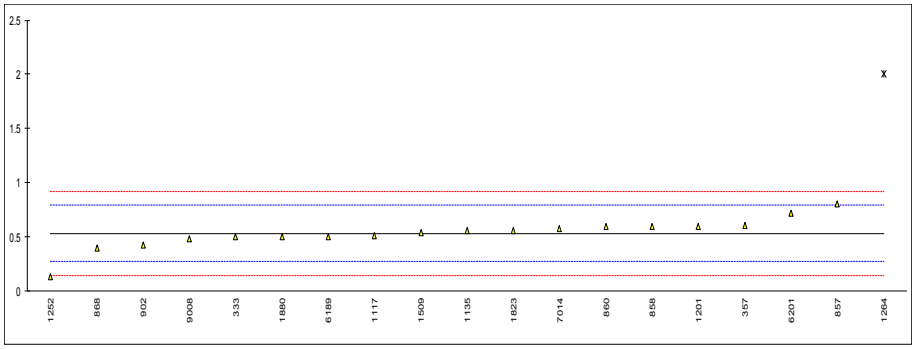


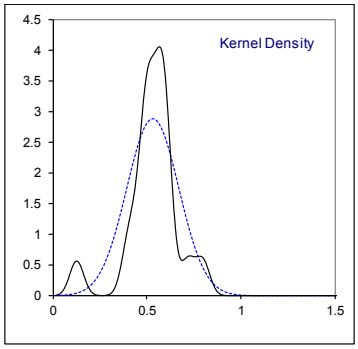
Determination of Sulphur on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5453	<1.0		-----	
169		-----		-----	
171	D5453	<1.0		-----	
173		-----		-----	
273	D5453	<1		-----	
311	D5453	<1		-----	
323	D5453	<1		-----	
333	D5453	0.5		-0.27	
343	D5453	<1		-----	
347	D5453	<1		-----	
357	D7183	0.61		0.58	
446		-----		-----	
551	D5453	<1		-----	
613		-----		-----	
857	D3120	0.8		2.05	
858	D5453	0.6		0.51	
860	D3120	0.6		0.51	
863		-----		-----	
868	D5453	0.4		-1.04	
869		-----		-----	
902	D5453	0.43		-0.81	
913		-----		-----	
1067		-----	W	-----	first reported 2.5
1117	D5453	0.510		-0.19	
1135	D5453	0.56		0.20	
1169		-----		-----	
1201	D5453	0.60		0.51	
1252	D5623	0.13		-3.13	
1264	D5453	2.0	G(0.01)	11.32	
1509	D5453	0.54		0.04	
1515		-----		-----	
1823	D5453	0.56		0.20	
1880	D5453	0.5		-0.27	
1935		-----		-----	
6189	D5453	0.5		-0.27	
6201	D5453	0.72		1.43	
6202		-----		-----	
7014	D5453	0.58		0.35	
9008	D5453	0.48		-0.42	
9014		-----		-----	

normality	not OK
n	18
outliers	1
mean (n)	0.534
st.dev. (n)	0.1386
R(calc.)	0.388
st.dev.(D5453:16e1)	0.1294
R(D5453:16e1)	0.362

application range method: 1-8000mg/kg

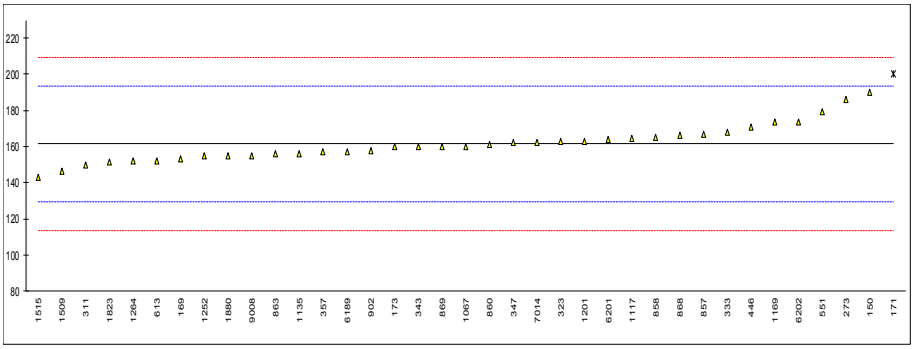


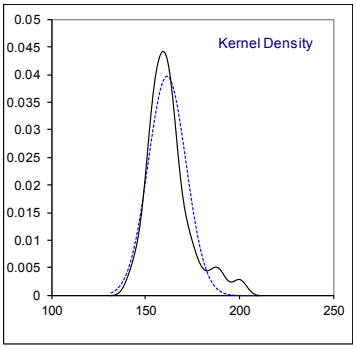


Determination of Water, coulometric KF titration on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	E1064	190		1.79	
169	D6304	153		-0.54	
171	E1064	200	R(0.05)	2.41	
173	D6304	160		-0.10	
273	E203	186		1.53	
311	E1064	150		-0.72	
323	E1064	163		0.09	
333	D6304	168		0.41	
343	E1064	160		-0.10	
347	E1064	162		0.03	
357	E1064	157		-0.29	
446	E1064	171		0.59	
551	E1064	179.1		1.10	
613	E203	152.3		-0.58	
857	E1064	167		0.34	
858	E1064	165		0.22	
860	E1064	161		-0.03	
863	E1064	156		-0.35	
868	E1064	166		0.28	
869	E1064	160		-0.10	
902	D7375	157.8		-0.24	
913		-----		-----	
1067	E1064	160		-0.10	
1117	E1064	164.3		0.17	
1135	E1064	156		-0.35	
1169	E1064	173.5		0.75	
1201	E1064	163		0.09	
1252	D1364	155		-0.41	
1264	E1064	152		-0.60	
1509	E1064	146.4		-0.95	
1515	E1064	143	C	-1.16	first reported 115
1823	E1064	151.4		-0.64	
1880	E1064	155		-0.41	
1935		-----		-----	
6189	E1064	157.0		-0.29	
6201	E1064	164		0.15	
6202	D6304	173.8		0.77	
7014	E1064	162.06		0.03	
9008	E1064	155		-0.41	
9014		-----		-----	

normality	suspect
n	36
outliers	1
mean (n)	161.55
st.dev. (n)	10.049
R(calc.)	28.14
st.dev.(E1064:16)	15.935
R(E1064:16)	44.62

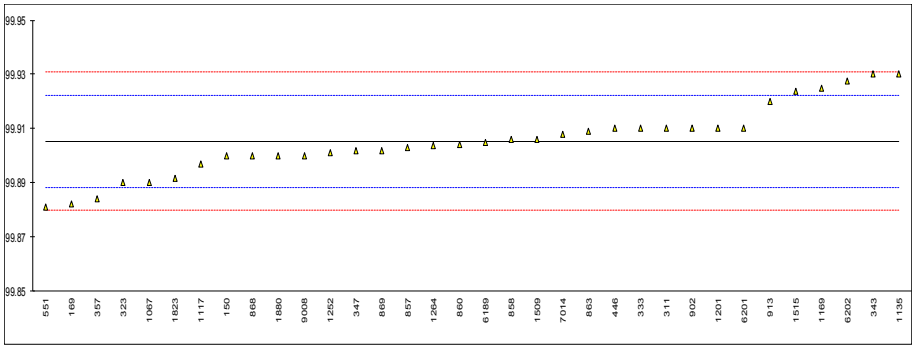


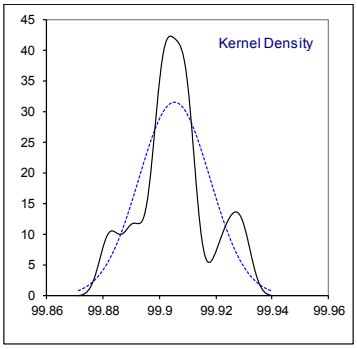


Determination of Purity by GC on sample #18190; results in %M/M

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5135	99.90		-0.63	
169	D5135	99.882		-2.73	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	99.91		0.55	
323	D5135	99.89		-1.80	
333	D5135	99.91		0.55	
343	D5135	99.93		2.89	
347	D5135	99.902		-0.39	
357	D5135	99.884		-2.50	
446	D5135	99.91		0.55	
551	D5135	99.881		-2.85	
613		-----		-----	
857	D5135	99.903		-0.27	
858	D5135	99.906		0.08	
860	D5135	99.904		-0.16	
863	D5135	99.909		0.43	
868	D5135	99.90		-0.63	
869	D5135	99.902		-0.39	
902	D5135	99.91		0.55	
913	D5135	99.92		1.72	
1067	In house	99.89		-1.80	
1117	D5135	99.897		-0.98	
1135	D5135	99.93		2.89	
1169	D5135	99.925		2.30	
1201	D5135	99.91		0.55	
1252	D5135	99.901		-0.51	
1264	D5135	99.9038		-0.18	
1509	D5135	99.906		0.08	
1515	D5135	99.9237		2.15	
1823	D5135	99.8918		-1.59	
1880	D5135	99.90		-0.63	
1935		-----		-----	
6189	D5135	99.905		-0.04	
6201	D5135	99.91		0.55	
6202	D5135	99.9277		2.62	
7014	D5135	99.908		0.31	
9008	D5135	99.90		-0.63	
9014		-----		-----	

normality	OK
n	34
outliers	0
mean (n)	99.9053
st.dev. (n)	0.01266
R(calc.)	0.0354
st.dev.(D5135:16e1)	0.00853
R(D5135:16e1)	0.0239

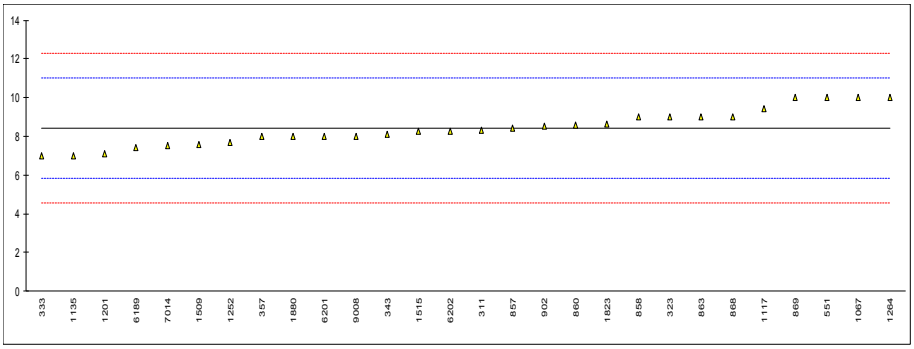


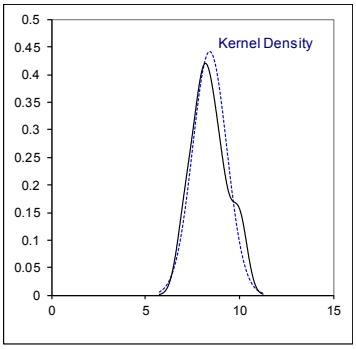


Determination of Benzene on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5135	<10		-----	
169	D5135	<10		-----	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D6229	8.3		-0.09	
323	D5135	9		0.45	
333	D5135	7		-1.10	
343	INH-1456	8.08		-0.26	
347		-----		-----	
357	D5135	8		-0.33	
446	D5135	<10		-----	
551	D5135	10		1.23	
613		-----		-----	
857	D5135	8.4		-0.02	
858	D5135	9		0.45	
860	D5135	8.6		0.14	
863	D5135	9		0.45	
868	D5135	9		0.45	
869	D5135	10.		1.23	
902	INH-123	8.5		0.06	
913	D5135	<10	C	-----	reported <0.0010 mg/kg (unit error?)
1067	In house	10		1.23	
1117	D5135	9.4		0.76	
1135	D5135	7		-1.10	
1169		-----		-----	
1201	In house	7.1		-1.02	
1252	D5135	7.7		-0.56	
1264	D5135	10		1.23	
1509	In house	7.6		-0.64	
1515	INH-2922	8.25		-0.13	
1823	INH-2922	8.65	C	0.18	first reported 13.6
1880	D4534	8.0		-0.33	
1935		-----		-----	
6189	D5135	7.4		-0.79	
6201	D5135	8		-0.33	
6202	D5135	8.26		-0.12	
7014	D5135	7.52		-0.70	
9008	D5135	8		-0.33	
9014		-----		-----	

normality	OK
n	28
outliers	0
mean (n)	8.42
st.dev. (n)	0.905
R(calc.)	2.53
st.dev.(D5135:16e1)	1.289
R(D5135:16e1)	3.61

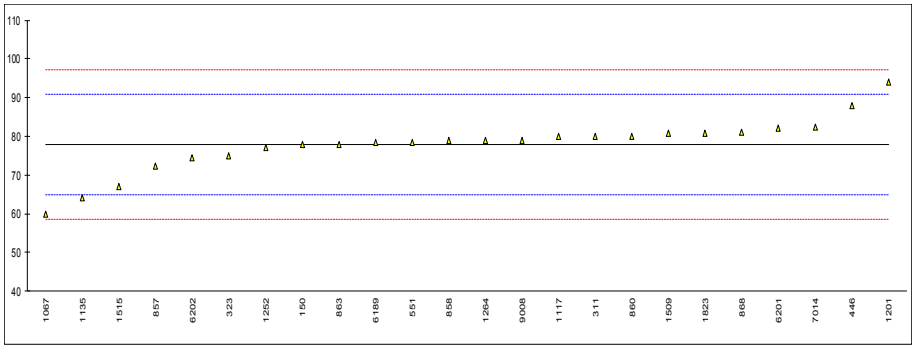


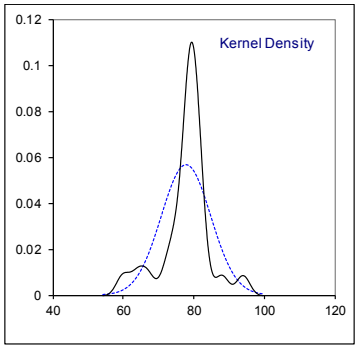


Determination of Toluene on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5135	78		0.02	
169		-----		-----	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	80		0.33	
323	D5135	75		-0.44	
333		-----		-----	
343		-----		-----	
347		-----		-----	
357		-----		-----	
446	D5135	88		1.57	
551	D5135	78.5		0.10	
613		-----		-----	
857	D5135	72.2		-0.87	
858	D5135	79		0.18	
860	D5135	80		0.33	
863	D5135	78	C	0.02	first reported 8
868	D5135	81		0.49	
869		-----		-----	
902		-----		-----	
913		-----		-----	
1067	In house	60		-2.76	
1117	D5135	79.95		0.33	
1135	D5135	64		-2.14	
1169		-----		-----	
1201	D5135	94		2.50	
1252	D5135	77		-0.13	
1264	D5135	79		0.18	
1509	D5135	80.7		0.44	
1515	D5135	67		-1.68	
1823	D5135	80.9		0.47	
1880		-----		-----	
1935		-----		-----	
6189	D5135	78.4		0.09	
6201	D5135	82		0.64	
6202	D5135	74.30		-0.55	
7014	D5135	82.26		0.68	
9008	D5135	79		0.18	
9014		-----		-----	

normality	not OK
n	24
outliers	0
mean (n)	77.84
st.dev. (n)	7.002
R(calc.)	19.61
st.dev.(Horwitz)	6.467
R(Horwitz)	18.11

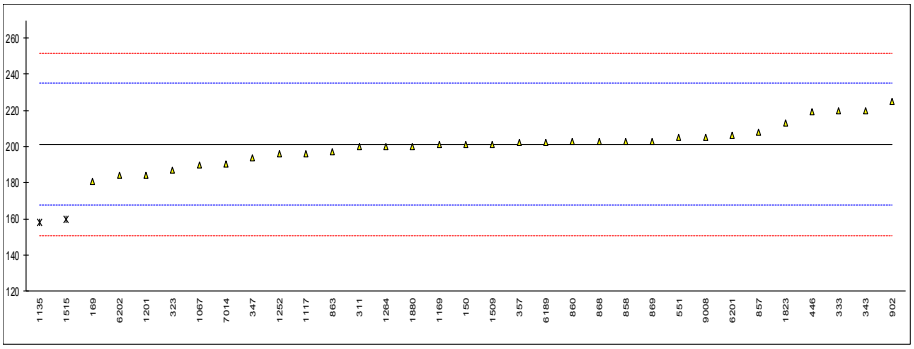


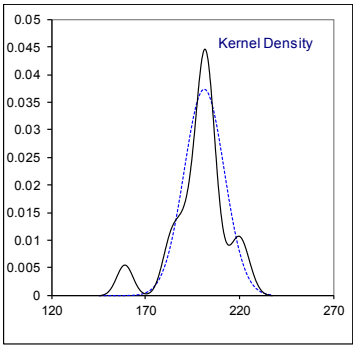


Determination of Ethylbenzene on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5135	201		-0.02	
169	D5135	180.8		-1.22	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	200		-0.08	
323	D5135	187		-0.85	
333	D5135	220		1.11	
343	D5135	220		1.11	
347	D5135	194		-0.44	
357	D5135	202		0.04	
446	D5135	219		1.05	
551	D5135	204.9		0.21	
613		-----		-----	
857	D5135	208.2		0.41	
858	D5135	203		0.10	
860	D5135	203		0.10	
863	D5135	197		-0.26	
868	D5135	203		0.10	
869	D5135	203		0.10	
902	D5135	225	C	1.41	first reported 261
913		-----		-----	
1067	In house	190		-0.67	
1117	D5135	196.33		-0.30	
1135	D5135	158	R(0.05)	-2.58	
1169	D5135	200.9		-0.02	
1201	D5135	184		-1.03	
1252	D5135	196		-0.32	
1264	D5135	200		-0.08	
1509	D5135	201.4		0.01	
1515	D5135	160	R(0.05)	-2.46	
1823	D5135	213.1		0.70	
1880	D5135	200		-0.08	
1935		-----		-----	
6189	D5135	202.3		0.06	
6201	D5135	206		0.28	
6202	D5135	183.95		-1.03	
7014	D5135	190.52		-0.64	
9008	D5135	205		0.22	
9014		-----		-----	

normality	OK
n	31
outliers	2
mean (n)	201.30
st.dev. (n)	10.680
R(calc.)	29.90
st.dev.(D5135:16e1)	16.783
R(D5135:16e1)	46.99

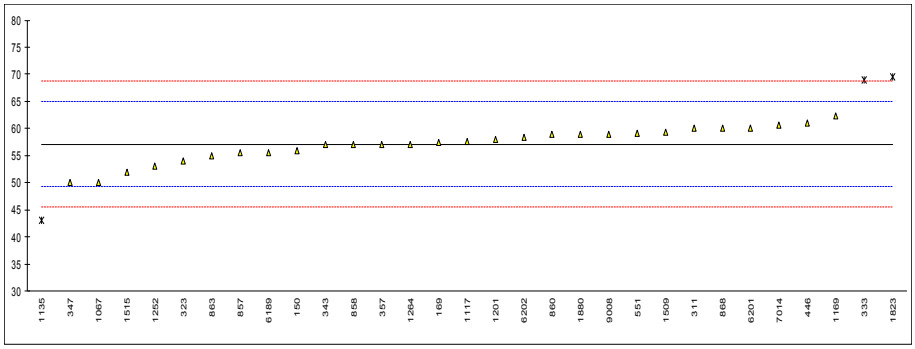


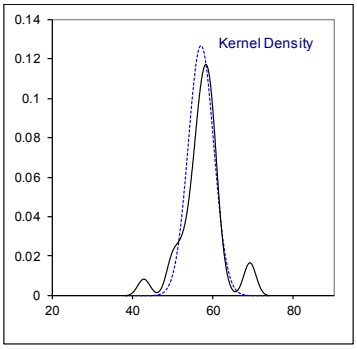


Determination of m- + p-Xylene on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5135	56		-0.29	
169	D5135	57.4		0.07	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	60		0.74	
323	D5135	54		-0.81	
333	D5135	69	R(0.05)	3.06	
343	D5135	57		-0.04	
347	D5135	50		-1.84	
357	D5135	57		-0.04	
446	D5135	61		0.99	
551	D5135	59.2		0.53	
613		-----		-----	
857	D5135	55.5		-0.42	
858	D5135	57		-0.04	
860	D5135	59		0.48	
863	D5135	55		-0.55	
868	D5135	60		0.74	
869		-----		-----	
902		-----		-----	
913		-----		-----	
1067	In house	50		-1.84	
1117	D5135	57.71		0.15	
1135	D5135	43	R(0.05)	-3.64	
1169	D5135	62.4	C	1.36	first reported 33.9
1201	D5135	58		0.22	
1252	D5135	53		-1.07	
1264	D5135	57		-0.04	
1509	D5135	59.3		0.56	
1515	D5135	52		-1.32	
1823	D5135	69.5	R(0.05)	3.18	
1880	D5135	59		0.48	
1935		-----		-----	
6189	D5135	55.5		-0.42	
6201	D5135	60		0.74	
6202	D5135	58.30		0.30	
7014	D5135	60.58		0.89	
9008	D5135	59		0.48	
9014		-----		-----	

normality	OK
n	28
outliers	3
mean (n)	57.14
st.dev. (n)	3.147
R(calc.)	8.81
st.dev.(D5135:16e1)	3.882
R(D5135:16e1)	10.87

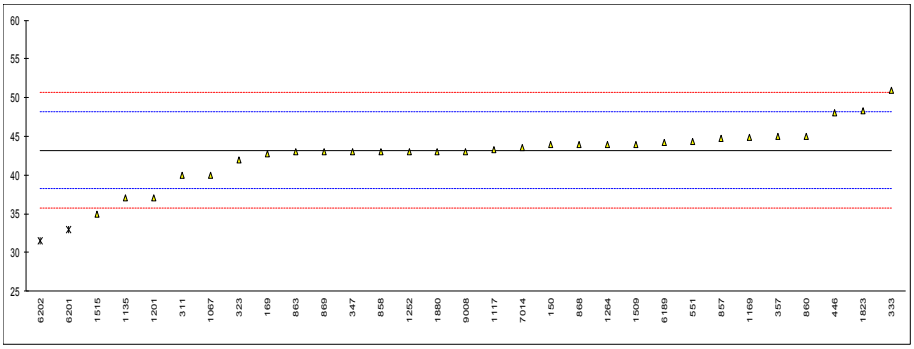


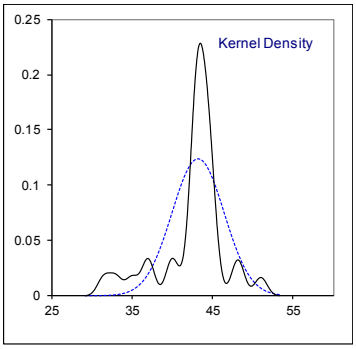


Determination of iso-Propylbenzene (Cumene) on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5135	44	C	0.32	first reported 29
169	D5135	42.8		-0.16	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	40		-1.28	
323	D5135	42		-0.48	
333	D5135	51		3.12	
343		-----		-----	
347	D5135	43	C	-0.08	first reported 28
357	D5135	45		0.72	
446	D5135	48		1.92	
551	D5135	44.3		0.44	
613		-----		-----	
857	D5135	44.7		0.60	
858	D5135	43		-0.08	
860	D5135	45		0.72	
863	D5135	43		-0.08	
868	D5135	44		0.32	
869	D5135	43		-0.08	
902		-----		-----	
913		-----		-----	
1067	In house	40		-1.28	
1117	D5135	43.29		0.03	
1135	D5135	37	C	-2.48	first reported 32
1169	D5135	44.9		0.68	
1201	D5135	37		-2.48	
1252	D5135	43		-0.08	
1264	D5135	44		0.32	
1509	D5135	44.0		0.32	
1515	D5135	35		-3.28	
1823	D5135	48.3		2.04	
1880	D5135	43		-0.08	
1935		-----		-----	
6189	D5135	44.2		0.40	
6201	D5135	33	C,DG(0.05)	-4.08	first reported 31
6202	D5135	31.50	DG(0.05)	-4.68	
7014	D5135	43.48		0.11	
9008	D5135	43		-0.08	
9014		-----		-----	
				-----	

normality	suspect
n	29
outliers	2
mean (n)	43.21
st.dev. (n)	3.234
R(calc.)	9.06
st.dev.(D5135:16e1)	2.501
R(D5135:16e1)	7.00

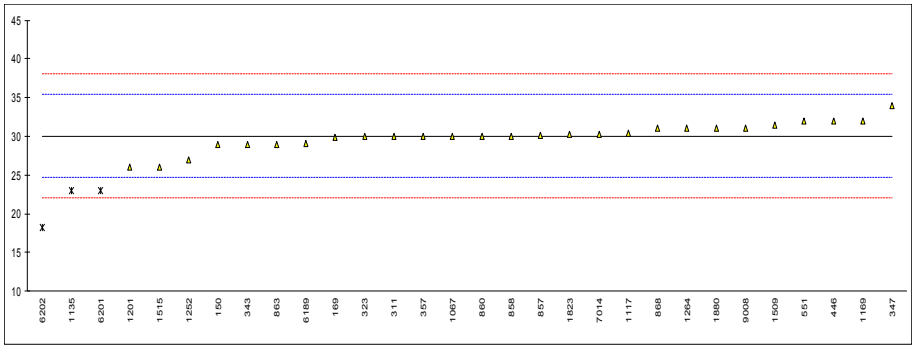


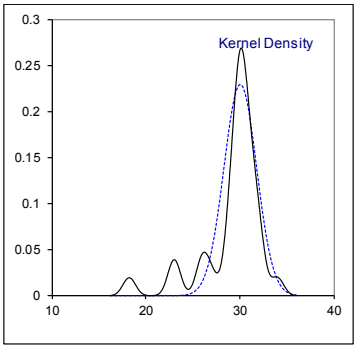


Determination of o-Xylene on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5135	29	C	-0.39	first reported 44
169	D5135	29.8		-0.09	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	30		-0.02	
323	D5135	30		-0.02	
333	D5135	<10	C	<-7.47	first reported 40, possibly a false negative test result?
343	D5135	29		-0.39	
347	D5135	34		1.47	
357	D5135	30		-0.02	
446	D5135	32		0.73	
551	D5135	32.0		0.73	
613		-----		-----	
857	D5135	30.1		0.02	
858	D5135	30		-0.02	
860	D5135	30		-0.02	
863	D5135	29		-0.39	
868	D5135	31		0.35	
869		-----		-----	
902		-----		-----	
913		-----		-----	
1067	In house	30		-0.02	
1117	D5135	30.39		0.13	
1135	D5135	23	R(0.05)	-2.63	
1169	D5135	32.0		0.73	
1201	D5135	26		-1.51	
1252	D5135	27		-1.14	
1264	D5135	31		0.35	
1509	D5135	31.4		0.50	
1515	D5135	26		-1.51	
1823	D5135	30.24	C	0.07	first reported 38.2
1880	D5135	31		0.35	
1935		-----		-----	
6189	D5135	29.1		-0.35	
6201	D5135	23	R(0.05)	-2.63	
6202	D5135	18.2	C,R(0.01)	-4.42	first reported 15.25
7014	D5135	30.28		0.09	
9008	D5135	31		0.35	
9014		-----		-----	

normality	suspect
n	27
outliers	3
mean (n)	30.05
st.dev. (n)	1.744
R(calc.)	4.88
st.dev.(D5135:16e1)	2.683
R(D5135:16e1)	7.51

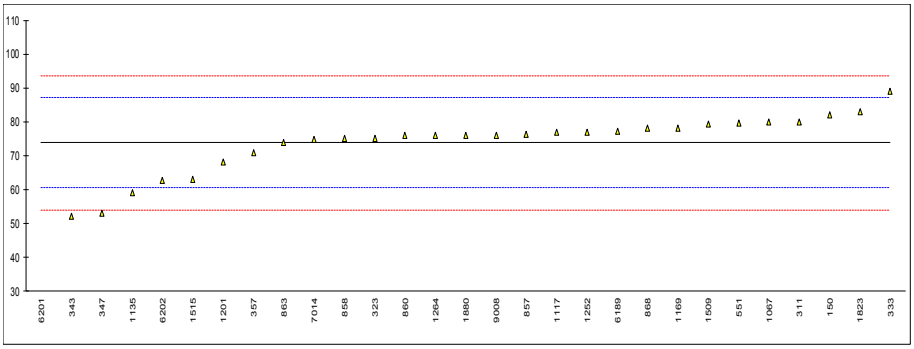


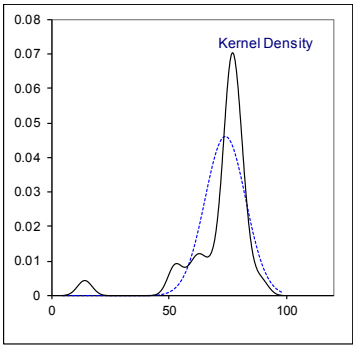


Determination of n-Propylbenzene on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5135	82		1.24	
169		-----		-----	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	80		0.93	
323	D5135	75		0.18	
333	D5135	89		2.30	
343	D5135	52		-3.31	
347	D5135	53		-3.16	
357	D5135	71		-0.43	
446		-----		-----	
551	D5135	79.6		0.87	
613		-----		-----	
857	D5135	76.2		0.36	
858	D5135	75		0.18	
860	D5135	76		0.33	
863	D5135	74		0.02	
868	D5135	78		0.63	
869		-----		-----	
902		-----		-----	
913		-----		-----	
1067	In house	80		0.93	
1117	D5135	76.78		0.45	
1135	D5135	59		-2.25	
1169	D5135	78.2		0.66	
1201	D5135	68		-0.89	
1252	D5135	77		0.48	
1264	D5135	76		0.33	
1509	D5135	79.2		0.81	
1515	D5135	63		-1.64	
1823	D5135	82.9		1.37	
1880	D5135	76		0.33	
1935		-----		-----	
6189	D5135	77.2		0.51	
6201	D5135	14	C,R(0.01)	-9.08	first reported 13
6202	D5135	62.85		-1.67	
7014	D5135	74.72		0.13	
9008	D5135	76		0.33	
9014		-----		-----	

normality	suspect
n	28
outliers	1
mean (n)	73.84
st.dev. (n)	8.654
R(calc.)	24.23
st.dev.(D5135:16e1)	6.593
R(D5135:16e1)	18.46

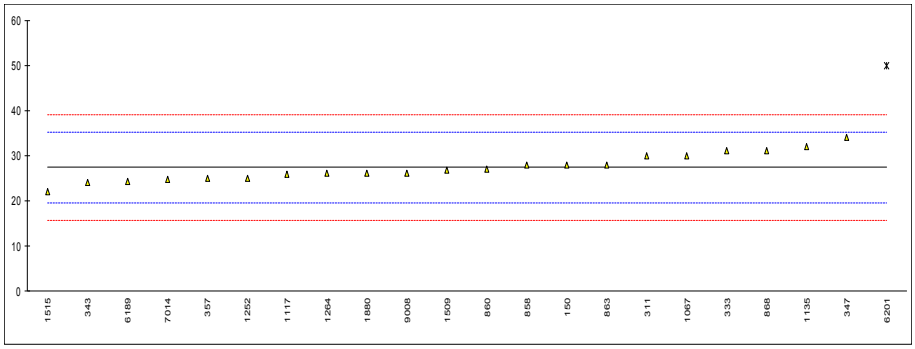


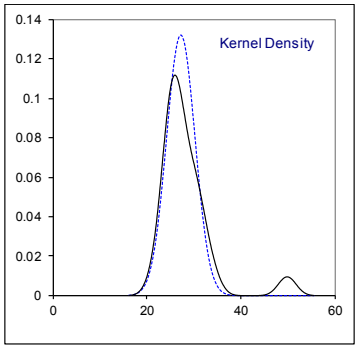


Determination of m- + p-Ethyltoluene on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5135	28		0.16	
169		-----		-----	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	30		0.67	
323		-----		-----	
333	D5135	31		0.93	
343	D5135	24		-0.86	
347	D5135	34	C	1.70	first reported 10
357	D5135	25		-0.61	
446		-----		-----	
551		-----		-----	
613		-----		-----	
857		-----		-----	
858	D5135	28		0.16	
860	D5135	27		-0.09	
863	D5135	28		0.16	
868	D5135	31		0.93	
869		-----		-----	
902		-----		-----	
913		-----		-----	
1067	In house	30		0.67	
1117	D7504	25.95		-0.36	
1135	D5135	32		1.19	
1169		-----		-----	
1201		-----		-----	
1252	D5135	25		-0.61	
1264	D5135	26		-0.35	
1509	D5135	26.7		-0.17	reported only p-Ethyltoluene
1515	D5135	22		-1.37	
1823		-----		-----	
1880	D5135	26		-0.35	
1935		-----		-----	
6189	D5135	24.3		-0.78	
6201	D5135	50	C,G(0.01)	5.79	first reported 40
6202		-----		-----	
7014	D5135	24.72		-0.68	
9008	D5135	26		-0.35	
9014		-----		-----	

normality	OK
n	21
outliers	1
mean (n)	27.37
st.dev. (n)	3.024
R(calc.)	8.47
st.dev.(D5135:16e1)	3.907
R(D5135:16e1)	10.94

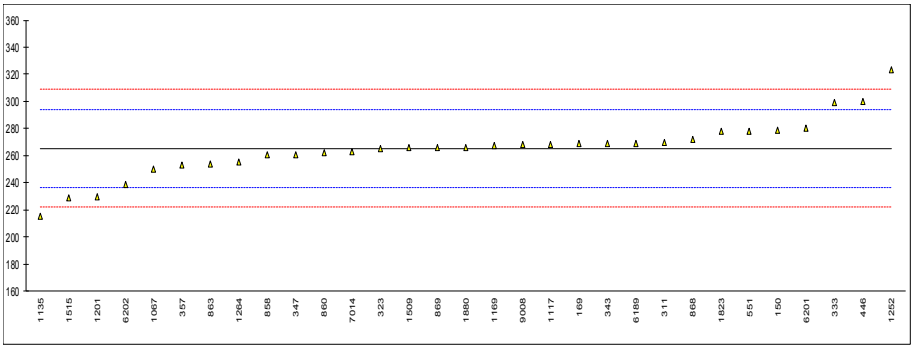


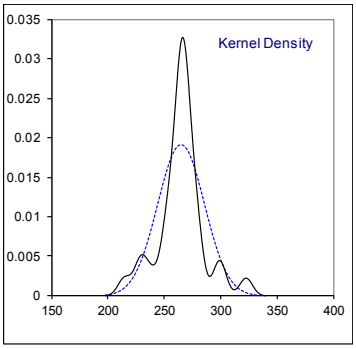


Determination of α-Methylstyrene on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5135	279		0.95	
169	D5135	268.9		0.25	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	270		0.33	
323	D5135	265		-0.02	
333	D5135	299		2.33	
343	D5135	269		0.26	
347	D5135	261		-0.30	
357	D5135	253		-0.85	
446	D5135	300		2.40	
551	D5135	278		0.88	
613		-----		-----	
857		-----		-----	
858	D5135	261		-0.30	
860	D5135	262		-0.23	
863	D5135	254		-0.78	
868	D5135	272		0.46	
869	D5135	266		0.05	
902		-----		-----	
913		-----		-----	
1067	In house	250		-1.06	
1117	D5135	268.5		0.22	
1135	D5135	215	C	-3.47	first reported 172
1169	D5135	267.1		0.13	
1201	D5135	230		-2.44	
1252	D5135	323		3.99	
1264	D5135	255		-0.71	
1509	D5135	265.6		0.02	
1515	D5135	229		-2.51	
1823	D5135	277.8		0.86	
1880	D5135	266		0.05	
1935		-----		-----	
6189	D5135	269.0		0.26	
6201	D5135	280		1.02	
6202	D5135	239.00		-1.82	
7014	D5135	262.9		-0.16	
9008	D5135	268		0.19	
9014		-----		-----	

normality	suspect
n	31
outliers	0
mean (n)	265.28
st.dev. (n)	20.799
R(calc.)	58.24
st.dev.(D5135:16e1)	14.476
R(D5135:16e1)	40.53





Determination of 1,2-Diethylbenzene on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150		-----		-----	
169		-----		-----	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	<10		-----	
323		-----		-----	
333		-----		-----	
343		-----		-----	
347		-----		-----	
357		-----		-----	
446		-----		-----	
551		-----		-----	
613		-----		-----	
857		-----		-----	
858		-----		-----	
860		-----		-----	
863		-----		-----	
868		-----		-----	
869		-----		-----	
902		-----		-----	
913		-----		-----	
1067		-----		-----	
1117	D5135	2.08		-----	
1135		-----		-----	
1169		-----		-----	
1201	D5135	10		-----	
1252	D5135	ND		-----	
1264		-----		-----	
1509		-----		-----	
1515	D5135	2	C	-----	reported 0.0002 mg/kg (unit error?)
1823		-----		-----	
1880		-----		-----	
1935		-----		-----	
6189		-----		-----	
6201		-----		-----	
6202		-----		-----	
7014		-----		-----	
9008		-----		-----	
9014		-----		-----	

normality	n.a.
n	4
outliers	0
mean (n)	<10
st.dev. (n)	n.a.
R(calc.)	n.a.
st.dev.(lit)	n.a.
R(lit)	n.a.

Determination of sum of α-Methylstyrene and 1,2-Diethylbenzene on sample #18190; results in mg/kg

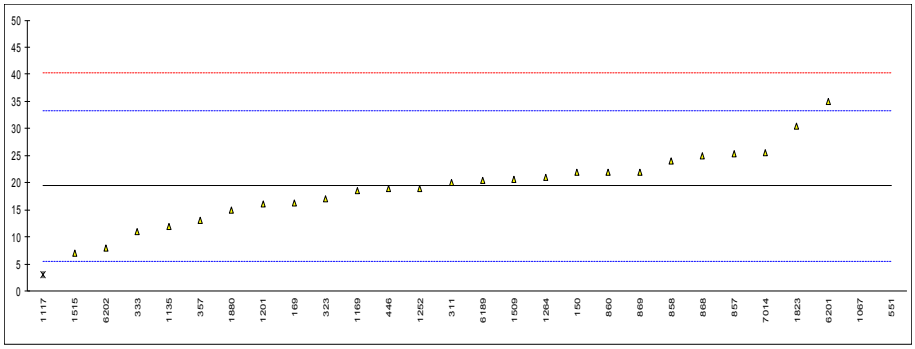
lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150		-----		-----	
169		-----		-----	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	270		-----	
323		-----		-----	
333		-----		-----	
343		-----		-----	
347		-----		-----	
357		-----		-----	
446		-----		-----	
551		-----		-----	
613		-----		-----	
857		-----		-----	
858		-----		-----	
860		-----		-----	
863		-----		-----	
868		-----		-----	
869		-----		-----	
902		-----		-----	
913		-----		-----	
1067		-----		-----	
1117	D5135	270.58		-----	
1135		-----		-----	
1169		-----		-----	
1201	D5135	240		-----	
1252	D5135	323		-----	
1264		-----		-----	
1509		-----		-----	
1515	D5135	231		-----	
1823		-----		-----	
1880		-----		-----	
1935		-----		-----	
6189		-----		-----	
6201		-----		-----	
6202		-----		-----	
7014		-----		-----	
9008		-----		-----	
9014		-----		-----	

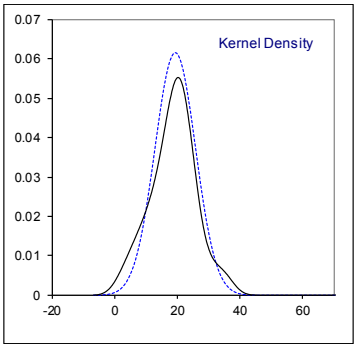
normality	unknown
n	5
outliers	0
mean (n)	266.92
st.dev. (n)	35.996
R(calc.)	100.79
st.dev.(D5135:16e1)	(14.506)
R(D5135:16e1)	(40.62)

Determination of Phenylacetylene on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5135	22		0.37	
169	D5135	16.2		-0.46	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	20		0.09	
323	D5135	17		-0.35	
333	D5135	11		-1.21	
343		-----		-----	
347		-----		-----	
357	D5135	13		-0.92	
446	D5135	19		-0.06	
551	D5135	115.1	R(0.01)	13.81	
613		-----		-----	
857	D5135	25.3		0.85	
858	D5135	24		0.66	
860	D5135	22		0.37	
863		-----		-----	
868	D5135	25		0.81	
869	D5135	22		0.37	
902		-----		-----	
913		-----		-----	
1067	In house	80	ex	8.74	excluded, see § 4.1
1117	D5135	3.11	ex	-2.35	excluded, see § 4.1
1135	D5135	12		-1.07	
1169	D5135	18.6		-0.12	
1201	D5135	16		-0.49	
1252	D5135	19		-0.06	
1264	D5135	21		0.23	
1509	D5135	20.7		0.19	
1515	D5135	7		-1.79	
1823	D5135	30.4		1.59	
1880	D5135	15		-0.64	
1935		-----		-----	
6189	D5135	20.5		0.16	
6201	D5135	35		2.25	
6202	D5135	8.05		-1.64	
7014	D5135	25.46		0.87	
9008		-----		-----	
9014		-----		-----	

normality	OK
n	25
outliers	1 (+2 ex)
mean (n)	19.41
st.dev. (n)	6.491
R(calc.)	18.18
st.dev.(D5135:16e1)	6.932
R(D5135:16e1)	19.41

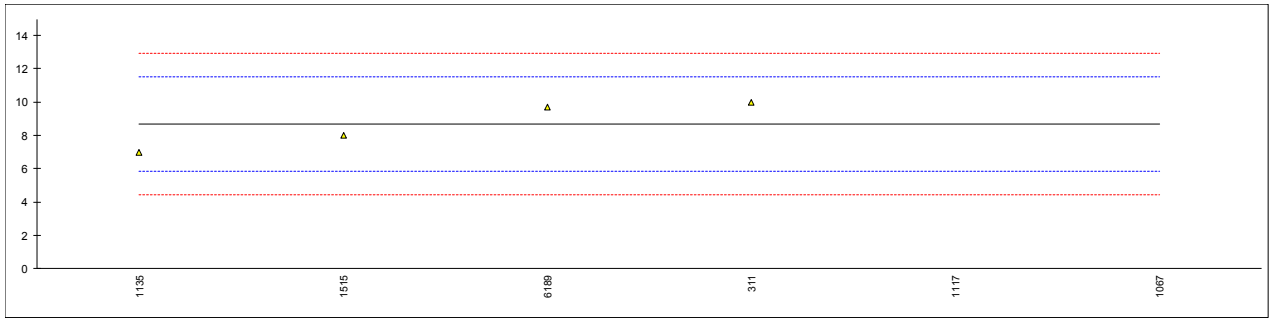




Determination of 3/4-Methylstyrenes on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150		-----		-----	
169		-----		-----	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	10		0.93	
323		-----		-----	
333		-----		-----	
343		-----		-----	
347		-----		-----	
357		-----		-----	
446		-----		-----	
551		-----		-----	
613		-----		-----	
857		-----		-----	
858		-----		-----	
860		-----		-----	
863		-----		-----	
868		-----		-----	
869		-----		-----	
902		-----		-----	
913		-----		-----	
1067	In house	40	ex	22.09	excluded, see § 4.1
1117	D5135	28.68	ex	14.11	excluded, see § 4.1
1135	D5135	7		-1.18	
1169		-----		-----	
1201	D5135	<10		-----	
1252	D5135	ND		-----	
1264		-----		-----	
1509		-----		-----	
1515	D5135	8		-0.48	
1823		-----		-----	
1880		-----		-----	
1935		-----		-----	
6189	D5135	9.7		0.72	
6201		-----		-----	
6202		-----		-----	
7014		-----		-----	
9008		-----		-----	
9014		-----		-----	

normality	unknown
n	4
outliers	0 (+2 ex)
mean (n)	8.68
st.dev. (n)	1.422
R(calc.)	3.98
st.dev.(Horwitz (n=2))	1.418
R(Horwitz (n=2))	3.97



Determination of sum of Phenylacetylene and 3/4-Methylstyrenes on sample #18190; results in mg/kg

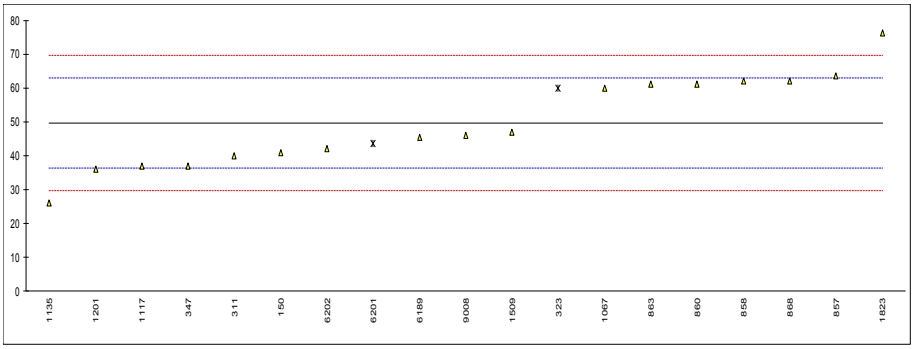
lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150		-----		-----	
169		-----		-----	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	30		-----	
323		-----		-----	
333		-----		-----	
343		-----		-----	
347		-----		-----	
357		-----		-----	
446		-----		-----	
551		-----		-----	
613		-----		-----	
857		-----		-----	
858		-----		-----	
860		-----		-----	
863		-----		-----	
868		-----		-----	
869		-----		-----	
902		-----		-----	
913		-----		-----	
1067	In house	110	ex	-----	excluded, see § 4.1
1117	D5135	29.79	ex	-----	excluded, see § 4.1
1135	D5135	19		-----	
1169		-----		-----	
1201	D5135	16		-----	
1252	D5135	19		-----	
1264		-----		-----	
1509		-----		-----	
1515	D5135	15		-----	
1823		-----		-----	
1880		-----		-----	
1935		-----		-----	
6189	D5135	30.2		-----	
6201		-----		-----	
6202		-----		-----	
7014		-----		-----	
9008		-----		-----	
9014		-----		-----	

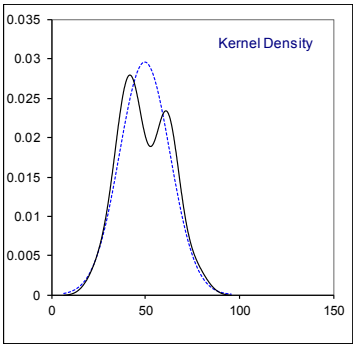
		unknow
	normality	n
	n	6
	outliers	0 (+2 ex)
	mean (n)	21.53
	st.dev. (n)	6.825
	R(calc.)	19.11
	st.dev.(Horwitz (n= 3))	(3.760)
	R(Horwitz (n= 3))	(10.53)

Determination Determination of Benzaldehyde on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5135	41		-1.29	
169		-----		-----	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	40		-1.44	
323	D5135	60	ex	1.57	excluded, see § 4.1
333		-----		-----	
343		-----		-----	
347	D5135	37		-1.90	
357		-----		-----	
446		-----		-----	
551		-----		-----	
613		-----		-----	
857	D5135	63.6		2.11	
858	D5135	62		1.87	
860	D5135	61		1.72	
863	D5135	61		1.72	
868	D5135	62		1.87	
869		-----		-----	
902		-----		-----	
913		-----		-----	
1067	In house	60		1.57	
1117	D5135	36.89		-1.91	
1135	D5135	26		-3.55	
1169		-----		-----	
1201	D5135	36		-2.05	
1252	D5135	ND		-----	
1264		-----		-----	
1509	D5135	47.0		-0.39	
1515		-----		-----	
1823	D5135	76.1		3.99	
1880		-----		-----	
1935		-----		-----	
6189	D5135	45.4		-0.63	
6201	D5135	43.6	ex	-0.90	excluded, see § 4.1
6202	D5135	42.18		-1.12	
7014		-----		-----	
9008	D5135	46		-0.54	
9014		-----		-----	

normality	OK
n	17
outliers	0 (+2 ex)
mean (n)	49.60
st.dev. (n)	13.450
R(calc.)	37.66
st.dev.(D5135:16e1)	6.643
R(D5135:16e1)	18.60

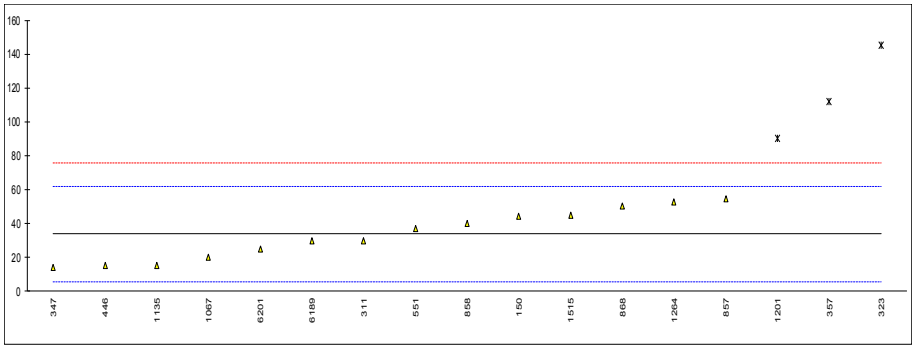


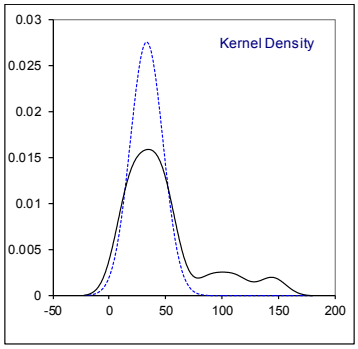


Determination of Nonaromatics on sample #18190; results in mg/kg

lab	method	value	mark	z(targ)	remarks
131		-----		-----	
150	D5135	44		0.73	
169		-----		-----	
171		-----		-----	
173		-----		-----	
273		-----		-----	
311	D5135	30		-0.26	
323	D5135	145	G(0.05)	7.92	
333		-----		-----	
343		-----		-----	
347	D5135	14		-1.40	
357	D5135	112	G(0.05)	5.57	
446	D5135	15		-1.33	
551	D5135	36.7		0.21	
613		-----		-----	
857	D5135	54.6		1.49	
858	D5135	40		0.45	
860		-----		-----	
863		-----		-----	
868	D5135	50		1.16	
869		-----		-----	
902		-----		-----	
913		-----		-----	
1067	In house	20		-0.98	
1117		-----	W	-----	first reported 389
1135	D5135	15		-1.33	
1169		-----		-----	
1201	D5135	90	G(0.05)	4.01	
1252	D5135	ND		-----	
1264	D5135	53		1.37	
1509		-----		-----	
1515	D5135	45		0.80	
1823		-----		-----	
1880		-----		-----	
1935		-----		-----	
6189	D5135	29.7		-0.29	
6201	D5135	25		-0.62	
6202		-----		-----	
7014		-----		-----	
9008		-----		-----	
9014		-----		-----	

normality	OK
n	14
outliers	3
mean (n)	33.714
st.dev. (n)	14.5126
R(calc.)	40.635
st.dev.(D5135:16e1)	14.0476
R(D5135:16e1)	39.333





APPENDIX 2

Number of participants per country

1 lab in	AUSTRALIA
2 labs in	BELGIUM
1 lab in	BRAZIL
1 lab in	CANADA
7 labs in	CHINA, People's Republic
2 labs in	FINLAND
1 lab in	FRANCE
1 lab in	INDIA
1 lab in	INDONESIA
1 lab in	IRAN, Islamic Republic of
2 labs in	KUWAIT
5 labs in	NETHERLANDS
1 lab in	SAUDI ARABIA
2 labs in	SINGAPORE
1 lab in	SOUTH AFRICA
2 labs in	SPAIN
2 labs in	TURKEY
1 lab in	UNITED ARAB EMIRATES
1 lab in	UNITED KINGDOM
6 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
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

1 iis Interlaboratory Studies, Protocol for the Organisation, Statistics & Evaluation, June 2018
2 ASTM E178:02
3 ASTM E1301:03
4 ISO13528:15
5 ISO 5725:86
6 ISO 5725, parts 1-6, 1994
7 M. Thompson and R. Wood, J. AOAC Int, 76, 926, (1993)
8 W.J. Youden and E.H. Steiner, Statistical Manual of the AOAC, (1975)
9 IP 367:84
10 DIN 38402 T41/42
11 P.L. Davies, Fr. Z. Anal. Chem, 331, 513, (1988)
12 J.N. Miller, Analyst, 118, 455, (1993)
13 Analytical Methods Committee Technical brief, No 4 January 2001.
14 P.J. Lothian and M. Thompson, The Royal Society of Chemistry, Analyst, 127, 1359-1364 (2002)
15 Bernard Rosner, Percentage Points for a Generalized ESD Many-Outlier Procedure, Technometrics, 25(2), 165-172, (1983)
16 Horwitz, R. Albert, J. AOAC Int. 79-3, 589 (1996)