Results of Proficiency Test
Benzene & Toluene
March 2017

Organised by: Institute for Interlaboratory Studies (iis)
Spijkenisse Netherlands

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1 INTRODUCTION

Since 1999, the Institute for Interlaboratory Studies (iis) organizes proficiency tests for the analysis of Benzene and Toluene every year. During the annual proficiency testing program 2016/2017, it was decided to continue the round robins for the analysis of Benzene in accordance with the latest applicable version of the specification for Benzene: ASTM D2359 and Toluene in accordance with the latest applicable version of the specification for Toluene: ASTM D841.
In the interlaboratory studies for Benzene 59 laboratories in 25 different countries and for Toluene 41 participants in 21 countries did register for participation. See appendix 2 for the number of participants per country. In this report, the results of the 2017 proficiency tests Benzene and Toluene 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, depending on the registration, to send one sample of Benzene (1 litre bottle, labelled #17020) and/or one sample of Toluene (1 litre bottle, labelled #17021). 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

BENZENE

The necessary bulk material of Benzene was obtained from a local chemical supplier. The approximately 70 kg of Benzene was spiked with 1001.9 mg 1-Methyl-2-Pyrrolidinone (for the Nitrogen determination), 510.1 mg o-Chlorotoluene (for the Organic Chlorides determination), 7003.2 mg Toluene and 2162.2 mg Methylcyclohexane. After homogenisation, 68 amber glass bottles of 1 litre were filled and labelled #17020. The homogeneity of the subsamples #17020 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 #17020-1	0.87895	120	2.2
sample #17020-2	0.87899	110	2.2
sample #17020-3	0.87897	110	2.2
sample #17020-4	0.87897	110	2.2
sample #17020-5	0.87897	120	2.2
sample #17020-6	0.87896	110	2.2
sample #17020-7	0.87897	110	2.2
sample #17020-8	0.87894	110	2.2

Table 1: homogeneity test results of Benzene subsamples #17020

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)	0.00004	13.0	0.00
Reference test method	ISO12185:96	ASTM 4492:10	ASTM D4629:12
0.3*R (reference test method)	0.00015	15.7	0.31

Table 2: evaluation of repeatabilities of subsamples #17020

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.

TOLUENE

The necessary bulk material of Toluene was purchased from a local chemical supplier. The approximately 60 litre, after homogenisation, was divided over 58 brown glass bottles of 1 litre and labelled #17021. The homogeneity of the subsamples #17021 was checked by determination of Density at 20°C, according to ISO12185 on 8 stratified randomly selected samples.

Toluene	Density at 20°C in kg/L
sample #17021-1	0.86509
sample #17021-2	0.86512
sample #17021-3	0.86512
sample #17021-4	0.86510
sample #17021-5	0.86509
sample #17021-6	0.86510
sample #17021-7	0.86511
sample #17021-8	0.86512

Table 3: homogeneity test results of Toluene subsamples #17021

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

	Density at 20°C in kg/L
r (observed)	0.00004
Reference test method	ISO12185:96
0.3*R (reference test method)	0.00015

Table 4: evaluation of repeatability of subsamples #17021

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

Depending on their registration to each of the participating laboratories one 1 litre bottle of Benzene labelled #17020 and/or one 1 litre bottle of Toluene labelled #17021 was sent on February 15, 2017. An SDS was added to the sample package.

2.5 STABILITY OF THE SAMPLES

The stabilities of Benzene and Toluene, packed in amber glass bottles, were checked. The materials were found sufficiently stable for the period of the proficiency test.

2.6 ANALYSES

The participants were requested to determine on the Benzene sample #17020: 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 and Solidification Point.
On Toluene sample #17021 was requested: Acid Wash Color, Appearance, Color Pt-Co, Copper Corrosion, Density at 20°C, Distillation, Purity, Benzene, Nonaromatics and Refractive Index.

It was explicitly requested to treat the samples as if they were routine samples 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	good
1 <	|z|	< 2	satisfactory
2 <	|z|	< 3	questionable
3 <	|z|		unsatisfactory

4 Evaluation

In this interlaboratory study, some problems were encountered with dispatch of the samples. Participants in Brazil, Portugal, India, Iran, Saudi Arabia and Vietnam received the sample late or not at all. For samples #17020 (Benzene) and #17021 (Toluene), respectively seven and five participants did not report any test results and six other

laboratories (three for Benzene and three for Toluene) reported the test results after the final reporting date. Not all laboratories were able to perform all analyses requested. Finally, for sample #17020 (Benzene) and sample #17021 (Toluene) in total 743 numerical test results were reported by 67 participants. Observed were 32 outlying results, which is 4.3% 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 SAMPLE AND TEST

In this section, the reported test results are discussed per sample and 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.

For Benzene sample #17020

Acid Wash Color: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in 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 #17020, 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 not problematic. Two statistical outliers were observed. The calculated reproducibility after rejection of the statistical outliers is in agreement with the requirements of ASTM D5194:13.
The average recovery of Organic Chloride (theoretical increment of 2.05 mg/kg) may be good: “less than <145%” (the actual blank is unknown).

Organic Chlorides: 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 D5808:09a(2014). The average recovery of Organic Chloride (theoretical increment of 2.05 mg/kg) may be good: “less than 141%” (the actual blank is unknown).

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 D1209:05e1(2011) and of ASTM D5386:16.

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 ISO12185:96.

Distillation: This determination was not problematic. In total seven statistical outliers were observed and three test results were excluded. However, all calculated reproducibilities after rejection of the suspect data is in agreement with the requirements of ASTM D850:11.
From the reported results of the 50% recovered, it appears that three participants 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. No statistical outliers were observed. The calculated reproducibility is in full agreement with the requirements of ASTM D4629:12.
The average recovery of Total Nitrogen (theoretical increment of 2.03 mg/kg) may be good: “less than 103%” (the actual blank is unknown).

Purity: This determination was problematic. Three statistical outliers were observed and one test result is excluded. The calculated reproducibility after rejection of the suspect data is not in agreement with the requirements of ASTM D4492:10.

Methylcyclohexane: This determination may not be problematic. No statistical outliers were observed. The calculated reproducibility is in almost agreement with the estimated reproducibility calculated using the Horwitz equation. The average recovery of Methylcyclohexane (theoretical increment of 30.97 mg/kg) may be good: “less than 124%” (the actual blank is unknown).
It is remarkable that twenty-four of the thirty-five laboratories used ASTM D4492, a method which may be not applicable for the determination of Methylcyclohexane, while only six laboratories used ASTM D5713 a method that is suitable for the determination of Methylcyclohexane in Benzene.

Toluene: This determination was not problematic. Three 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.
The average recovery of Toluene (theoretical increment of 100.32 mg/kg) may be good: “less than 103%” (the actual blank is unknown).

Nonaromatics: This determination was problematic. No statistical outliers were observed. However, the calculated reproducibility is not in agreement with the requirements of ASTM D4492:10.

Solidification Point: 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 D852:16.

For Toluene sample #17021

Acid Wash Color: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in 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.

Appearance: No analytical problems were observed. All labs agreed about the appearance of the sample #17021, which was bright, clear and free of suspended matter (Pass).

Color Pt-Co: 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 D5386:16 and of ASTM D1209:05e1(2011)

Copper Corrosion: No problems have been observed. All participants agreed on a result of 1, 1A or pass.

Density at 20°C: 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 ISO12185:96.

Distillation: This determination was problematic. In total four statistical outliers were observed.
For Initial Boiling Point (IBP), the calculated reproducibility of the after rejection of the statistical outlier is not in agreement with the requirements of D850:16. For 50% recovered, the calculated reproducibility after rejection of the statistical outliers is in agreement with the requirements of D850:16. For the Dry Point (DP) no comparison between the calculated reproducibility and the reproducibility of reference test method (D850:16) has been made. The reproducibility of the Dry Point of the reference method is most likely not applicable for sample #17021 due to the lower purity level of sample #17021.

Purity: Four test results were excluded. No comparison between the calculated reproducibility and the reproducibility of reference test method (D7504:16) has been made. The reproducibility of the reference method is based on a purity level much higher than the purity level of sample #17021.

Benzene: 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 D7504:16.

Nonaromatics: This determination may not be problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the estimated requirements of ASTM D2360:11. However in the literature the reproducibility is given at a concentration level which is far below the concentration level of sample #17021.

Refractive Index: This determination may not be problematic. One statistical outlier was observed. The calculated reproducibility after rejection of the statistical outlier is in agreement with the requirements of ASTM D1218:12.

4.2 PERFORMANCE EVALUATION FOR THE GROUP OF LABORATORIES

A comparison has been made between the reproducibility as declared by the relevant standard and the reproducibility as found for the group of participating laboratories. The average results per sample, 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	R (lit)
Acid Wash Color		40	0.8(1-)	0.7	2.1
Acidity	mg NaOH/100ml	38	NFA	n.a.	n.a.
Appearance		38	Pass	n.a.	n.a.
Bromine Index	mg Br/100g	41	1.7	2.1	4.6
Total Chlorides	mg/kg	9	3.0	1.7	0.9
Organic Chlorides	mg/kg	28	2.9	1.0	1.3
Color Pt-Co		32	4.5	3.4	7
Density at 20ºC	kg/L	42	0.8790	0.0002	0.0005
Distillation, IBP	°C	29	79.8	0.3	0.4
Distillation, 50% rec.	°C	30	80.1	0.1	0.4
Distillation, DP	°C	29	80.3	0.2	0.4
Total Nitrogen	mg/kg	31	2.09	1.02	1.03
Purity	%M/M	43	99.979	0.004	0.003
Methylcyclohexane	mg/kg	35	38.3	10.9	9.9
Toluene	mg/kg	46	104	19	48
Nonaromatics	mg/kg	46	102	65	38
Solidification Point	°C	24	5.49	0.03	0.05

Table 5: reproducibilities on Benzene sample #17020

Parameter	unit	n	average	2.8 *sd_R	R (lit)
Acid Wash Color		31	1.3 (1+)	1.3	2.3
Appearance		28	Pass	n.a.	n.a.
Color Pt-Co		25	4.9	3.0	5.4
Copper corrosion		24	1 (1A)	n.a.	n.a.
Density at 20ºC	kg/L	33	0.8651	0.0001	0.0005
Distillation, IBP	°C	27	109.5	1.0	0.6
Distillation, 50% rec.	°C	25	110.6	0.2	0.2
Distillation, DP	°C	27	113.6	2.9	(0.5) *)
Purity	%M/M	27	98.443	0.441	(0.013) *)
Benzene	mg/kg	29	290	76	40
Nonaromatics	mg/kg	27	10179	3362	4868
Refractive Index at 25°C		19	1.4928	0.0003	0.0005

Table 6: reproducibilities on Toluene sample #17021

*) purity of sample #17021 may be too low

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 standards. The tests that are problematic have been discussed in paragraph 4.1.

4.3 COMPARISON OF THE PROFICIENCY TEST OF MARCH 2017 WITH PREVIOUS PTS

	March 2017	March 2016	Feb 2015	Feb 2014	April 2013
Total Number of reporting labs	67	59	51	58	41
Number of results reported	743	793	729	800	686
Statistical outliers	32	19	15	36	27
Percentage outliers	4.3%	2.4%	2.1%	4.5%	3.9%

Table 7: 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 standards. The conclusions are given the following tables:

	March 2017	March 2016	Feb 2015	Feb 2014	April 2013
Acid Wash Color	++	++	++	n.e.	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 Chloride	+/-	+	+	++	--
Organic Chloride	+	++	++	++	+
Color Pt-Co	++	++	++	++	++
Density at 20ºC	++	++	++	++	++
Distillation, IBP	+	++	+	+/-	++
Distillation, 50%	++	++	++	+	++
Distillation, DP	++	+	+	--	+
Total Nitrogen	+/-	--	-	-	+/-
Purity	+/-	-	+/-	--	+
Methylcyclohexane	+/- *)	+/- *)	n.e.	n.e.	-- *)
Toluene	++	++	+	++	++
Nonaromatics	-	+/-	-	+	--
Solidification Point	+	+/-	+/-	--	+/-

Table 8: comparison determinations on Benzene against the standards

*) against the strict Horwitz equation

	March 2017	March 2016	Feb 2015	Feb 2014	April 2013
Acid Wash Color	+	++	++	+/-	n.e.
Appearance	n.e.	n.e.	n.e.	n.e.	n.e.
Color Pt-Co	+	++	+	++	++
Copper Corrosion	n.e.	n.e.	n.e.	n.e.	n.e
Density at 20 ºC	++	++	++	++	++
Distillation, IBP	-	+	++	++	-
Distillation, 50%	+/-	+	+	+	-
Distillation, DP	n.e. *)	+	-	--	++
Purity	n.e. *)	+	+	-	+/-
Benzene	--	+/- **)	+ **)	+/- **)	- **)
Nonaromatics	+	++	+	++	++
Refractive Index at 25°C	+	-	n.e.	n.e.	n.e.

Table 9: comparison determinations on Toluene against the standards

*) purity of sample #17021 is too low

**) against the strict Horwitz equation

The performance of the determinations against the requirements of the respective standards is listed in the above table. The following performance categories were used:

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

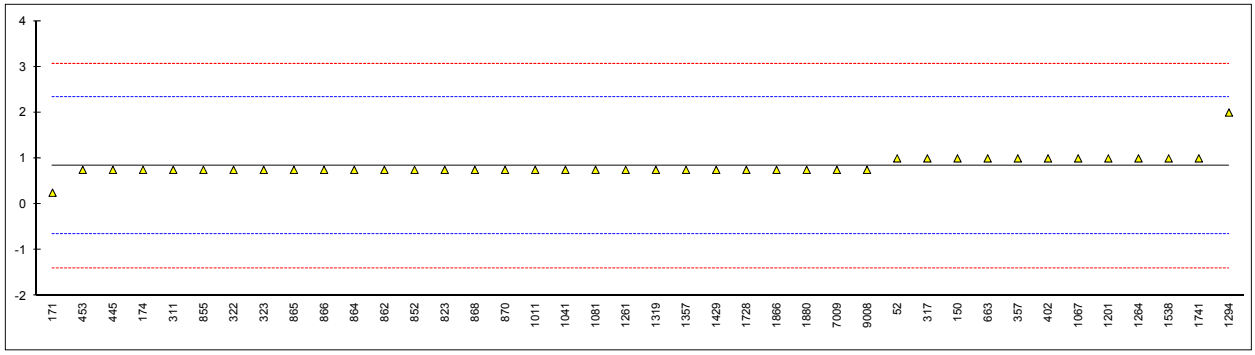
APPENDIX 1

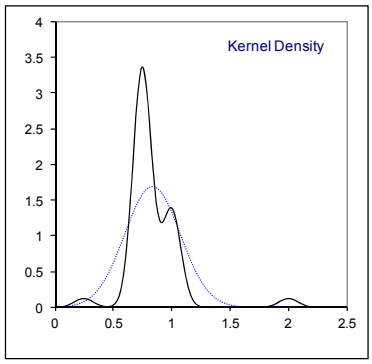
Determination of Acid Wash Color (acid layer) on Benzene sample #17020

lab	method	value	mark	z(targ)	remarks
52	D848	1		0.22	
150	D848	1		0.22	
171	D848	0+		-0.79	
174	D848	1-		-0.12	
311	D848	1-		-0.12	
317	D848	1		0.22	
322	D848	-1		-0.12	
323	D848	-1		-0.12	
334		-----		-----	
336		-----		-----	
347		-----		-----	
357	D848	1		0.22	
402	D848	1		0.22	
444		-----		-----	
445	D848	1-		-0.12	
453	D848	1-		-0.12	
551		-----		-----	
555		-----		-----	
663	D848	1		0.22	
823	D848	1-		-0.12	
852	D848	No.1-		-0.12	
855	D848	No.1-		-0.12	
862	D848	NO.1-		-0.12	
864	D848	No.1-		-0.12	
865	D848	No.1-		-0.12	
866	D848	No.1-		-0.12	
868	D848	No.1-		-0.12	
870	D848	No.1-		-0.12	
912		-----		-----	
913		-----		-----	
963		-----		-----	
1011	D848	1-		-0.12	
1040		-----		-----	
1041	D848	1-		-0.12	
1067	D848	1		0.22	
1081	D848	1-		-0.12	
1117		-----		-----	
1151		-----		-----	
1201	D848	1		0.22	
1261	D848	<1		-0.12	
1264	D848	1.0		0.22	
1291		-----		-----	
1294		2		1.56	
1307		-----		-----	
1319	D848	No.1-		-0.12	
1357	D848	<1		-0.12	
1429	D848	1-		-0.12	
1538	D848	1		0.22	
1728	D848	1-		-0.12	
1741	D848	1		0.22	
1781		-----		-----	
1790		-----		-----	
1812		-----		-----	
1823		-----		-----	
1846		-----		-----	
1866	D848	-1		-0.12	
1880	D848	<1		-0.12	
7009	D848	-1		-0.12	
9008	D848	-1		-0.12	

normality	not OK
n	40
outliers	0
mean (n)	0.84 (1-)
st.dev. (n)	0.237
R(calc.)	0.66
R(D848:14)	2.09

*) In the calculation of the mean, standard deviation, reproducibility and in the graphs, a reported value of ‘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).


4
3
2
1
0
-1
-2
171
453
445
174
311
855
322
323
865
866
864
862
852
823
868
870
1011
1041
1081
1261
1319
1357
1429
1728
1866
1880
7009
9008
52
317
150
663
357
402
1067
1201
1264
1538
1741
1294


Kernel Density
4
3.5
3
2.5
2
1.5
1
0.5
0
0
0.5
1
1.5
2
2.5

Determination of Acidity on Benzene sample #17020; results in mg NaOH per 100mL

lab	method	value	mark	z(targ)	remarks
52	D847	NIL		-----	
150	D847	No Free Acid		-----	
171	D847	0.2		-----	
174		-----		-----	
311	D847	pass		-----	
317		-----		-----	
322	D847	PASS		-----	
323	D847	NFANEOA		-----	
334		-----		-----	
336		-----		-----	
347	D847	No free acid		-----	
357	D847	No free acid		-----	
402		-----		-----	
444		-----		-----	
445	D847	No free acid		-----	
453	D847	pass		-----	
551		-----		-----	
555		-----		-----	
663	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		-----	
865	D847	No free acid		-----	
866	D847	Pass		-----	
868	D847	PASS		-----	
870	D847	No Free Acid		-----	
912		-----		-----	
913		-----		-----	
963		-----		-----	
1011	D847	Pass		-----	
1040		-----		-----	
1041		-----		-----	
1067	D847	Pass		-----	
1081	D847	0		-----	
1117	D847	0.16		-----	
1151		-----		-----	
1201	D847	nill		-----	
1261	D847	NFA		-----	
1264	D847	No Free Acid		-----	
1291		-----		-----	
1294		-----		-----	
1307		-----		-----	
1319	D847	0.0		-----	
1357	D847	NFA		-----	
1429	D847	No free acid		-----	
1538	D847	nfa		-----	
1728	D847	ABSENT		-----	
1741	D847	no free acid		-----	
1781		-----		-----	
1790		-----		-----	
1812		-----		-----	
1823	D847	No free acid		-----	
1846		-----		-----	
1866	D847	NFA		-----	
1880	D847	NFA		-----	
7009	D847	No Free Acid		-----	
9008	D847	NFA		-----	
	normality	n.a.			
	n	38			
	outliers	n.a.			
	mean (n)	No acid present			
	st.dev. (n)	n.a.			
	R(calc.)	n.a.			
	R(D847:15)	n.a.			

Abbreviation
NFA = No free acid
NFANEOA = No free acid, no evidence of acidity

Determination of Appearance on Benzene sample #17020

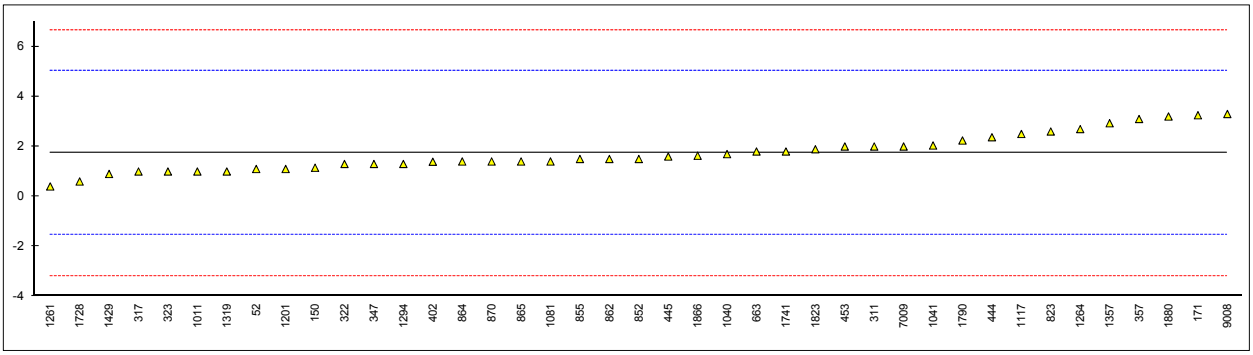
lab	method	value	mark	z(targ)	remarks
52	D4176	Pass		-----	
150	E2680	Pass		-----	
171	Visual	Clear and free from suspended matter		-----	
174	E2680	CFSM		-----	
311	INH-402	bright & clear		-----	
317	D4176	Pass		-----	
322	Visual	PASS		-----	
323	D4176	C&B		-----	
334		-----		-----	
336		-----		-----	
347	E2680	PASS		-----	
357	E2680	Pass		-----	
402		-----		-----	
444	E2680	Pass		-----	
445	E2680	Pass		-----	
453	Visual	clear & bright		-----	
551		-----		-----	
555		-----		-----	
663	Visual	B&C		-----	
823	E2680	Pass		-----	
852	E2680	Pass		-----	
855	E2680	Pass		-----	
862	E2680	Pass		-----	
864	Visual	Pass		-----	
865	E2680	Pass		-----	
866	E2680	Pass		-----	
868	E2680	PASS		-----	
870	E2680	Pass		-----	
912		-----		-----	
913		-----		-----	
963		-----		-----	
1011		-----		-----	
1040		Clear and bright	C	-----	Reported: clear, bright and visually free from solid matter and undissolved water at ambient temp. First reported 1.695
1041		-----		-----	
1067	E2680	Clear and Bright		-----	
1081		-----		-----	
1117	D4176	Pass		-----	
1151		-----		-----	
1201	D4176	Clear and bright		-----	
1261	Visual	Clear and Bright		-----	
1264	Visual	Clear		-----	
1291		-----		-----	
1294		-----		-----	
1307		-----		-----	
1319	Visual	Clear liquid free of sediment and haze		-----	
1357	E2680	C&B		-----	
1429	E2680	Clear + bright		-----	
1538	Visual	c&b		-----	
1728	Visual	CLEAR		-----	
1741		-----		-----	
1781		-----		-----	
1790		-----		-----	
1812		-----		-----	
1823	D4176	Clear/FFSM/No free water		-----	
1846		-----		-----	
1866		-----		-----	
1880	Visual	Pass		-----	
7009	Visual	Clear		-----	
9008	Visual	Clear liquid		-----	
	normality	n.a.			
	n	38			
	outliers	n.a.			
	mean (n)	Pass (C&B)			
	st.dev. (n)	n.a.			
	R(calc.)	n.a.			
	R(E2680:09)	n.a.			

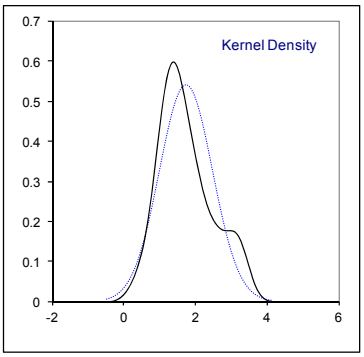
Abbreviations:
C&B / B&C = clear and bright / bright and clear
CFSM = clear and free from suspended matter
FFSM = free from suspended matter

Determination of Bromine Index on Benzene sample #17020; results in mg Br/100g

lab	method	Value	mark	z(targ)	remarks
52	D1492	1.1		-0.39	
150	D1492	1.15		-0.36	
171	D5776	3.25		0.92	
174		-----		-----	
311	D5776	2.0		0.16	
317	D5776	1.0		-0.45	
322	D5776	1.3		-0.27	
323	D5776	1.0		-0.45	
334		-----		-----	
336		-----		-----	
347	D5776	1.3		-0.27	
357	D5776	3.1		0.83	
402	D5776	1.39		-0.21	
444	D5776	2.37		0.38	
445	D2710	1.6		-0.08	
453	D1492	2		0.16	
551		-----		-----	
555		-----		-----	
663	D1492	1.8		0.04	
823	D1492	2.6		0.52	
852	D5776	1.5		-0.15	
855	D5776	1.5		-0.15	
862	D5776	1.5		-0.15	
864	D5776	1.4		-0.21	
865	D5776	1.4		-0.21	
866	D5776	<10		-----	
868	D5776	<10		-----	
870	D5776	1.4		-0.21	
912		-----		-----	
913		-----		-----	
963		-----		-----	
1011	D5776	1		-0.45	
1040	DIN51774	1.695	C	-0.03	First reported as Appearance
1041	DIN51774	2.04		0.18	
1067	DIN51774	< 10		-----	
1081	D1492	1.4		-0.21	
1117	D1492	2.5		0.46	
1151		-----		-----	
1201	D2710	1.1		-0.39	
1261	D1492	0.4		-0.81	
1264	D1492	2.696		0.58	
1291		-----		-----	
1294		1.3		-0.27	
1307		-----		-----	
1319	D5776	1.0		-0.45	
1357	D5776	2.93		0.73	
1429	D2710	0.9		-0.51	
1538	D1492	<1		-----	
1728	D5776	0.6		-0.69	
1741	UOP304	1.8		0.04	
1781		-----		-----	
1790	D5776	2.24		0.31	
1812		-----		-----	
1823	D1492	1.89		0.09	
1846		-----		-----	
1866	D5776	1.63		-0.07	
1880	D1492	3.2		0.89	
7009	D1492	2		0.16	
9008	D1492	3.3		0.95	

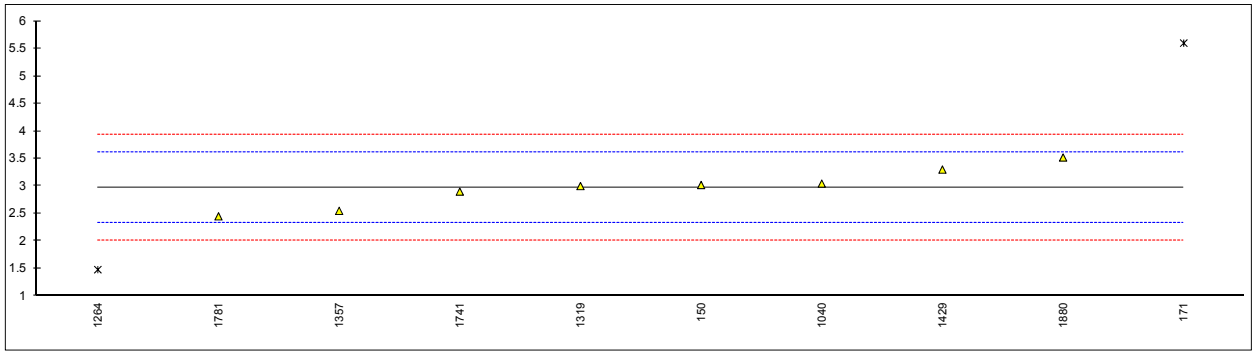
normality	OK
n	41
outliers	0
mean (n)	1.74
st.dev. (n)	0.739
R(calc.)	2.07
R(D5776:14a)	4.6

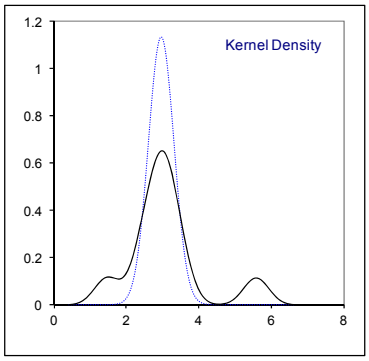

6
4
2
0
-2
-4
1261
1728
1429
317
323
1011
1319
52
1201
150
322
347
1294
402
864
870
865
1081
855
862
852
445
1866
1040
663
1741
1823
453
311
7009
1041
1790
444
1117
823
1264
1357
357
1880
171
9008


Kernel Density
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-2
0
2
4
6

Determination of Chlorides, Total on Benzene sample #17020; results in mg/kg

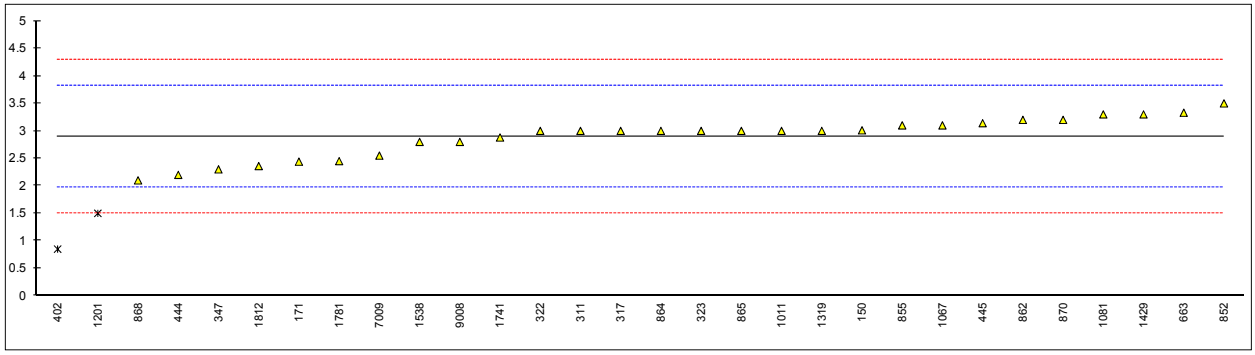
lab	method	value	mark	z(targ)	remarks
52		-----		-----	
150	D7359	3.02		0.15	
171	D5194	5.6	D(0.01)	8.17	
174		-----		-----	
311		-----		-----	
317		-----		-----	
322		-----		-----	
323		-----		-----	
334		-----		-----	
336		-----		-----	
347		-----		-----	
357		-----		-----	
402		-----		-----	
444		-----		-----	
445		-----		-----	
453		-----		-----	
551		-----		-----	
555		-----		-----	
663		-----		-----	
823		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
865		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
963		-----		-----	
1011		-----		-----	
1040	EN14077	3.045		0.22	
1041		-----		-----	
1067		-----		-----	
1081		-----		-----	
1117		-----		-----	
1151		-----		-----	
1201		-----		-----	
1261		-----		-----	
1264	D5194	1.48	D(0.05)	-4.65	
1291		-----		-----	
1294		-----		-----	
1307		-----		-----	
1319		3		0.08	
1357	UOP779	2.55	C	-1.32	First reported 1.29
1429	D7359	3.3		1.02	
1538		-----		-----	
1728		-----		-----	
1741		2.90		-0.23	
1781	INH-D3-S-708	2.45		-1.63	
1790		-----		-----	
1812		-----		-----	
1823		-----		-----	
1846		-----		-----	
1866		-----		-----	
1880	D7359	3.52	C	1.70	Was reported as organic Chlorides, used test method is for total Chlorides
7009	D4929&D7536	-----		-----	See test result in next table; used test method is for organic Chlorides
9008		-----		-----	
	normality	OK			
	n	8			
	outliers	2	Spike		
	mean (n)	2.973	2.05		Recovery < 145%
	st.dev. (n)	0.3530			
	R(calc.)	0.988			
	R(D5194:13)	0.9			

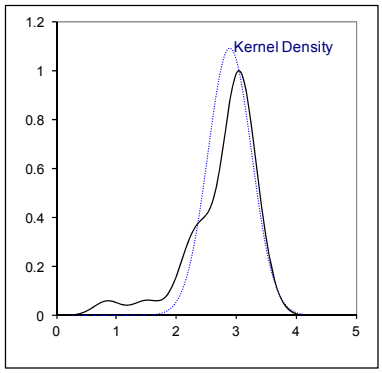

6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
1
1284
1781
1357
1741
1319
150
1040
1429
1880
171


Kernel Density
1.2
1
0.8
0.6
0.4
0.2
0
0
2
4
6
8

Determination of Chlorides, Organic on Benzene sample #17020; results in mg/kg

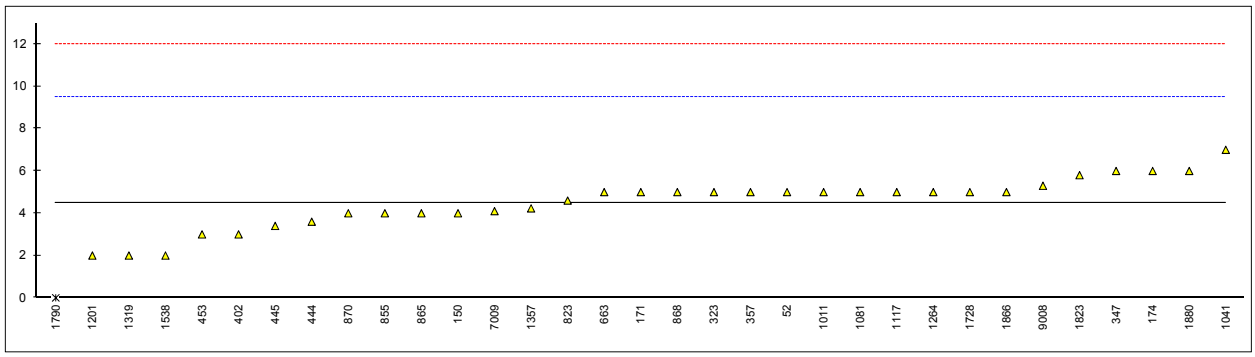
lab	method	value	mark	z(targ)	remarks
52		-----		-----	
150	D7359	3.01		0.25	
171	D5808	2.44		-0.98	
174		-----		-----	
311	D5808	3		0.23	
317	UOP779	3.0		0.23	
322	D5808	3.0		0.23	
323	D5808	3		0.23	
334		-----		-----	
336		-----		-----	
347	D4929B	2.3		-1.28	
357		-----		-----	
402	D5808	0.85	C,R(0.01)	-4.40	First reported 0.5
444	IP510	2.2		-1.50	
445	IP510	3.14		0.53	
453		-----		-----	
551		-----		-----	
555		-----		-----	
663	D5808	3.33		0.94	
823		-----		-----	
852	D5808	3.5		1.30	
855	UOP779	3.1		0.44	
862	D5808	3.2		0.66	
864	D5808	3.0		0.23	
865	D5808	3.0		0.23	
866		-----		-----	
868	D5808	2.1		-1.71	
870	D5808	3.2		0.66	
912		-----		-----	
913		-----		-----	
963		-----		-----	
1011	D5808	3		0.23	
1040		-----		-----	
1041		-----		-----	
1067	UOP779	3.1		0.44	
1081	D5808	3.3		0.87	
1117		-----		-----	
1151		-----		-----	
1201	D5808	1.5	C,R(0.05)	-3.00	First reported 1.3
1261		-----		-----	
1264		-----		-----	
1291		-----		-----	
1294		-----		-----	
1307		-----		-----	
1319	D5808	3		0.23	
1357		-----		-----	
1429	D7359	3.3		0.87	
1538	D5808	2.8		-0.20	
1728		-----		-----	
1741	D5808	2.88		-0.03	
1781	D5808	2.45		-0.96	
1790		-----		-----	
1812		2.36		-1.15	
1823		-----		-----	
1846		-----		-----	
1866		-----		-----	
1880	D7359	-----		-----	See test result in previous table; used test method is for total Chlorides
7009	D4929&D7536	2.55	C	-0.74	Was reported as total Chloride, used test method is for org. Chlorides
9008	D5808	2.8		-0.20	
	normality	OK			
	n	28			
	outliers	2	Spike		
	mean (n)	2.895	2.05		Recover < 141%
	st.dev. (n)	0.3658			
	R(calc.)	1.024			
	R(D5808:09a)	1.3			

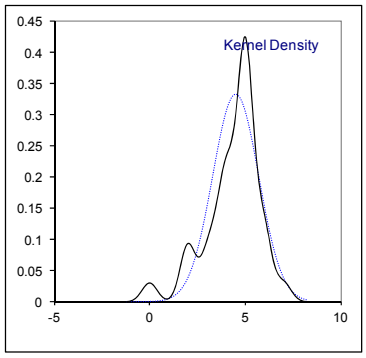

5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
402
1201
868
444
347
1812
171
1781
7009
1538
9008
1741
322
311
317
864
323
865
1011
1319
150
855
1067
445
862
870
1081
1429
663
852


Kernel Density
1.2
1
0.8
0.6
0.4
0.2
0
0
1
2
3
4
5

Determination of Color (Pt-Co scale) on Benzene sample #17020

lab	method	value	mark	z(targ)	remarks
52	D5386	5		0.20	
150	D5386	4		-0.20	
171	D1209	5		0.20	
174	D1209	6		0.60	
311	D1209	<5		-----	
317	D1209	<5		-----	
322	D1209	<5		-----	
323	D1209	5		0.20	
334		-----		-----	
336		-----		-----	
347	D5386	6		0.60	
357	D5386	5		0.20	
402	D1209	3		-0.60	
444	D5386	3.6		-0.36	
445	D1209	3.4		-0.44	
453	D1209	3		-0.60	
551		-----		-----	
555		-----		-----	
663	D1209	5		0.20	
823	D5386	4.6		0.04	
852	D1209	<5		-----	
855	D1209	4		-0.20	
862	D1209	<5		-----	
864	D1209	<5		-----	
865	D1209	4		-0.20	
866	D1209	<5		-----	
868	D1209	5		0.20	
870	D1209	4		-0.20	
912		-----		-----	
913		-----		-----	
963		-----		-----	
1011	D1209	5		0.20	
1040	ISO6271	<5		-----	
1041	ISO6271	7		1.00	
1067	D1209	< 5		-----	
1081	D5386	5		0.20	
1117	D1209	5		0.20	
1151		-----		-----	
1201	D1209	2		-1.00	
1261	D1209	<5		-----	
1264	D1209	5		0.20	
1291		-----		-----	
1294		-----		-----	
1307		-----		-----	
1319	D1209	2		-1.00	
1357	D1209	4.23		-0.11	
1429	D1209	Less than 5		-----	
1538	D1209	2		-1.00	
1728	D1209	5		0.20	
1741	ISO6271	<5		-----	
1781		-----		-----	
1790	D1209	0	R(0.05)	-1.80	
1812		-----		-----	
1823	D5386	5.8		0.52	
1846		-----		-----	
1866	D1209	5		0.20	
1880	D5386	6.0		0.60	
7009	D1209	4.1		-0.16	
9008	D5386	5.3		0.32	
	normality	OK			
	n	32			
	outliers	1			
	mean (n)	4.50			
	st.dev. (n)	1.203			
	R(calc.)	3.37			
	R(D1209:05)	7			Compare R(D5386:16) = 5.30

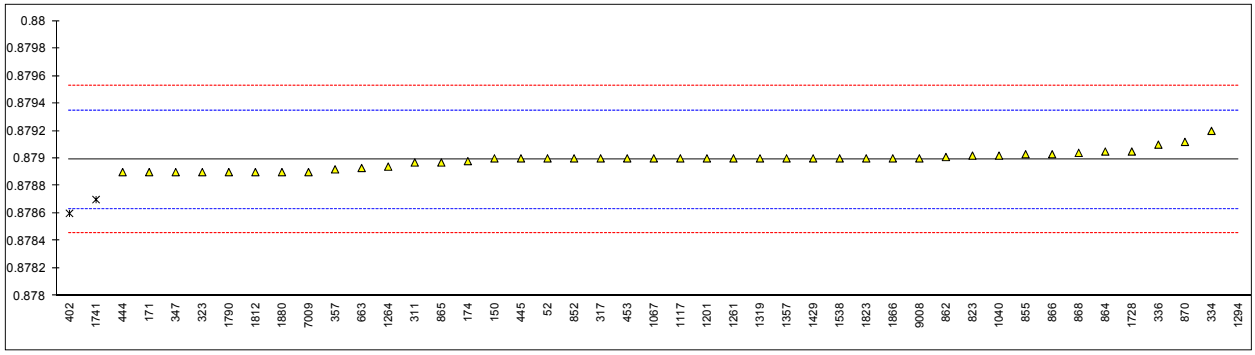

12
10
8
6
4
2
0
1790
1201
1319
1538
453
402
445
444
870
855
865
150
7009
1357
823
663
171
868
323
357
52
1011
1081
1117
1264
1728
1866
9008
1823
347
174
1880
1041

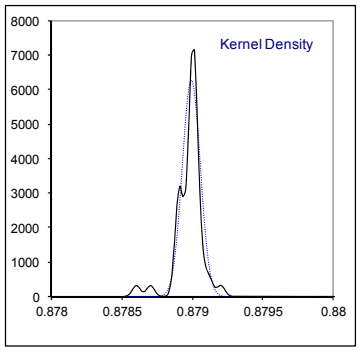

Kernel Density
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-5
0
5
10

Determination of Density at 20°C on Benzene sample #17020; results in kg/L

lab	method	value	mark	z(targ)	remarks
52	D4052	0.8790		0.06	
150	ISO12185	0.8790		0.06	
171	D4052	0.8789		-0.50	
174	D4052	0.87898		-0.06	
311	D4052	0.87897		-0.11	
317	D4052	0.8790		0.06	
322		-----		-----	
323	D4052	0.8789		-0.50	
334	ISO12185	0.8792		1.18	
336	ISO12185	0.8791		0.62	
347	D4052	0.8789		-0.50	
357	D4052	0.87892		-0.39	
402	D4052	0.8786	R(0.01)	-2.18	
444	D4052	0.8789		-0.50	
445	D4052	0.8790		0.06	
453	ISO12185	0.8790	C	0.06	First reported 879.0 kg/L
551		-----		-----	
555		-----		-----	
663	D4052	0.87893		-0.34	
823	ISO12185	0.87902		0.17	
852	D4052	0.8790		0.06	
855	D4052	0.87903		0.22	
862	D4052	0.87901		0.11	
864	D4052	0.87905		0.34	
865	D4052	0.87897		-0.11	
866	D4052	0.87903		0.22	
868	D4052	0.87904		0.28	
870	D4052	0.87912		0.73	
912		-----		-----	
913		-----		-----	
963		-----		-----	
1011		-----		-----	
1040	ISO12185	0.87902	C	0.17	First reported 879.02 kg/L
1041		-----		-----	
1067	D4052	0.8790		0.06	
1081		-----		-----	
1117	D4052	0.8790		0.06	
1151		-----		-----	
1201	D4052	0.8790		0.06	
1261	D4052	0.8790		0.06	
1264	D4052	0.87894		-0.28	
1291		-----		-----	
1294		0.88371	R(0.01)	26.43	
1307		-----		-----	
1319	D4052	0.8790		0.06	
1357	D4052	0.8790		0.06	
1429	D4052	0.8790		0.06	
1538	D4052	0.8790		0.06	
1728	ISO12185	0.87905		0.34	
1741	D4052	0.8787	R(0.01)	-1.62	
1781		-----		-----	
1790	D4052	0.8789		-0.50	
1812	ISO12185	0.8789		-0.50	
1823	D4052	0.879		0.06	
1846		-----		-----	
1866	ISO12185	0.8790		0.06	
1880	D4052	0.8789		-0.50	
7009	D4052	0.8789		-0.50	
9008	D4052	0.8790		0.06	

normality	suspect
n	42
outliers	3
mean (n)	0.87899
st.dev. (n)	0.000064
R(calc.)	0.00018
R(ISO12185:96)	0.0005


0.88
0.8798
0.8796
0.8794
0.8792
0.879
0.8788
0.8786
0.8784
0.8782
0.878
402 1741 444 171 347 323 1790 1812 1880 7009 357 663 1264 311 865 174 150 445 52 852 317 453 1067 1117 1201 1261 1319 1357 1429 1538 1823 1866 9008 862 823 1040 855 866 868 864 1728 336 870 334 1294


Kernel Density
8000
7000
6000
5000
4000
3000
2000
1000
0
0.878 0.8785 0.879 0.8795 0.88

Determination of Distillation on Benzene sample #17020; results in °C

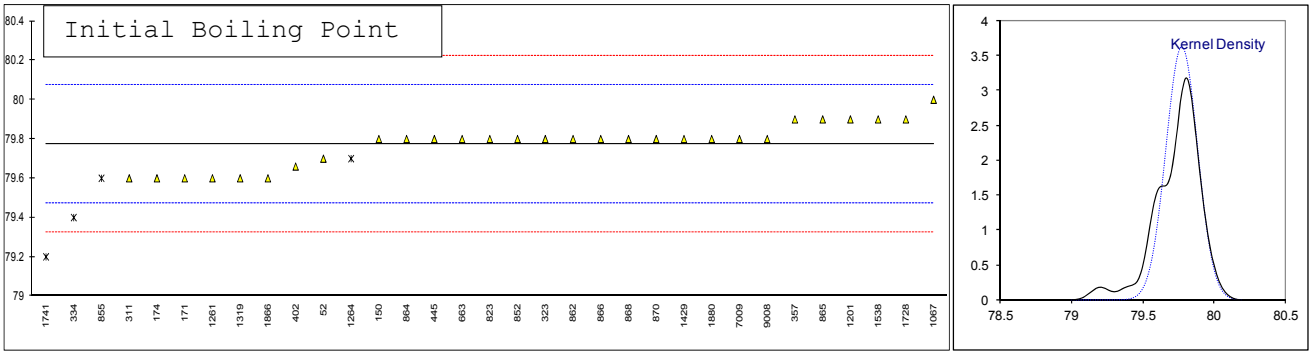
Lab	method	mode	IBP	mark	z(targ)	50%	mark	z(targ)	DP	mark	z(targ)
52	D850	Automated	79.7		-0.50	80.1		0.01	80.1		-1.03
150	D850	Automated	79.8		0.17	80.1		0.01	80.2		-0.36
171	D850	Automated	79.6		-1.16	80.0		-0.66	80.2		-0.36
174	D850	Automated	79.6		-1.16	80.2		0.68	80.3		0.31
311	D850	Automated	79.6		-1.16	80.1		0.01	80.3		0.31
317			-----		-----	-----		-----	-----		-----
322			-----		-----	-----		-----	-----		-----
323	D850	Manual	79.8		0.17	80.1		0.01	80.2		-0.36
334	D850	Automated	79.4	C, ex	-2.50	79.6	R(0.01)	-3.32	79.7	C,R(0.01)	-3.69
336			-----		-----	-----		-----	-----		-----
347		Automated	-----		-----	-----		-----	-----		-----
357	D850	Automated	79.9		0.84	80.1		0.01	80.2		-0.36
402	D850	Manual	79.66		-0.76	80.06		-0.26	80.26		0.04
444			-----		-----	-----		-----	-----		-----
445	D850	Manual	79.8		0.17	80.2		0.68	80.4		0.97
453			-----		-----	-----		-----	-----		-----
551			-----		-----	-----		-----	-----		-----
555			-----		-----	-----		-----	-----		-----
663	D850	Automated	79.8		0.17	80.1		0.01	80.2		-0.36
823	D850	Automated	79.8		0.17	80.1		0.01	80.2		-0.36
852	D850	Manual	79.8		0.17	80.1		0.01	80.2		-0.36
855	D850	Manual	79.6	ex	-1.16	79.9	R(0.01)	-1.32	80.0	R(0.05)	-1.69
862	D850	Manual	79.8		0.17	80.1		0.01	80.3		0.31
864	D850		79.8		0.17	80.1		0.01	80.2		-0.36
865	D850	Manual	79.9		0.84	80.1		0.01	80.3		0.31
866	D850	Manual	79.8		0.17	80.1		0.01	80.3		0.31
868	D850	Manual	79.8		0.17	80.1		0.01	80.3		0.31
870	D850	Manual	79.8		0.17	80.1		0.01	80.2		-0.36
912			-----		-----	-----		-----	-----		-----
913			-----		-----	-----		-----	-----		-----
963			-----		-----	-----		-----	-----		-----
1011			-----		-----	-----		-----	-----		-----
1040			-----		-----	-----		-----	-----		-----
1041			-----		-----	-----		-----	-----		-----
1067	D850	Manual	80.0		1.50	80.1		0.01	80.2		-0.36
1081			-----		-----	-----		-----	-----		-----
1117			-----		-----	-----		-----	-----		-----
1151			-----		-----	-----		-----	-----		-----
1201	D850	Automated	79.9		0.84	80.1		0.01	80.3		0.31
1261	D850	Automated	79.6		-1.16	80.1		0.01	80.3		0.31
1264	D850	Automated	79.7	ex	-0.50	80.4	R(0.01)	2.01	80.6	R(0.01)	2.31
1291			-----		-----	-----		-----	-----		-----
1294			-----		-----	-----		-----	-----		-----
1307			-----		-----	-----		-----	-----		-----
1319	D850	Manual	79.6		-1.16	80.0		-0.66	80.2		-0.36
1357			-----		-----	-----		-----	-----		-----
1429	D850	Automated	79.8		0.17	80.1		0.01	80.2		-0.36
1538	D850	Automated	79.9		0.84	80.1		0.01	80.4		0.97
1728	D850	Manual	79.9		0.84	80.1		0.01	80.3		0.31
1741	D850		79.2	R(0.01)	-3.83	80.0		-0.66	80.2		-0.36
1781			-----		-----	-----		-----	-----		-----
1790			-----		-----	-----		-----	-----		-----
1812			-----		-----	-----		-----	-----		-----
1823			-----		-----	-----		-----	-----		-----
1846			-----		-----	-----		-----	-----		-----
1866	D850	Automated	79.6		-1.16	80.1		0.01	-----		-----
1880	D850	Automated	79.8		0.17	80.2		0.68	80.3		0.31
7009			79.8		0.17	80.1		0.01	80.3		0.31
9008	D850	Automated	79.8		0.17	80.1		0.01	80.3		0.31
	normality		OK			not OK			OK		
	n		29			30			29		
	outliers		1 (+3 ex)			3			3		
	mean (n)		79.77			80.10			80.25		
	st.dev. (n)		0.110			0.046			0.068		
	R(calc.)		0.31			0.13			0.19		
	R(D850:16)		0.42			0.42			0.42		

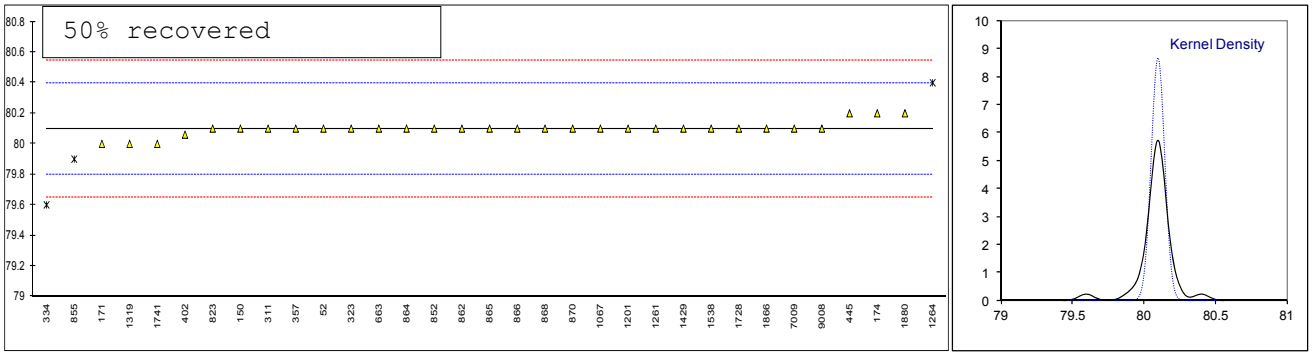
Lab 334: First reported IBP=79.2 and DP=79.6

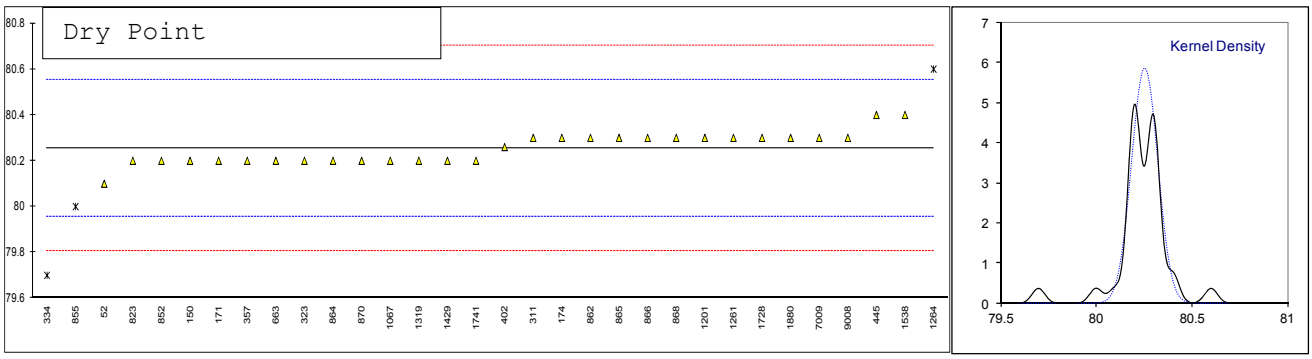
Theoretical mid boiling point = 80.1 °C

After manual correction:

334	D850	Automated	79.9	0.88	80.1	0.08	80.2	-0.35
855	D850	Manual	79.8	0.22	80.1	0.08	80.2	-0.35
1264	D850	Automated	79.4	-2.45	80.1	0.08	80.3	0.32
	normality		OK		not OK		OK	
	n		32		30		32	
	outliers		1		3		0	
	mean (n)		79.77		80.09		80.25	
	st.dev. (n)		0.126		0.031		0.067	
	R(calc.)		0.35		0.087		0.19	
	R(D850:16)		0.42		0.42		0.42	

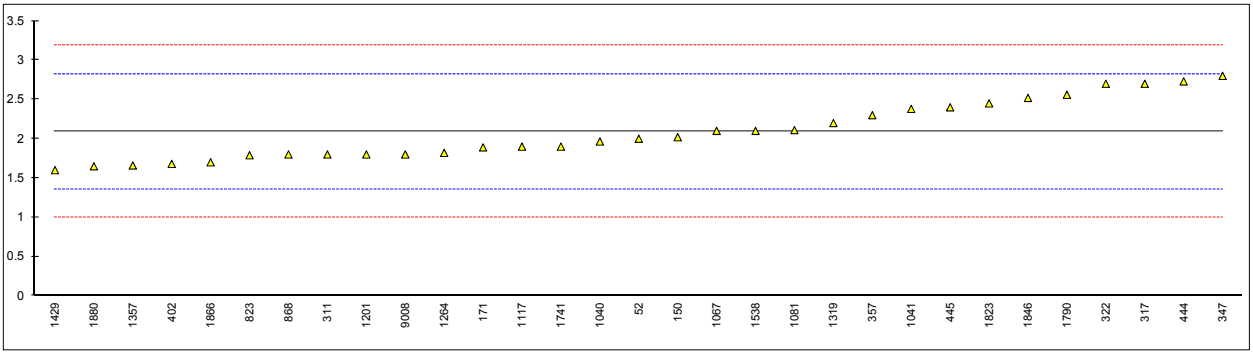


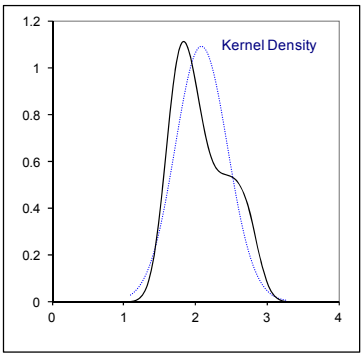




Determination of Total Nitrogen on Benzene sample #17020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D4629	2.0		-0.25	
150	D4629	2.02		-0.19	
171	D6069	1.89		-0.55	
174		-----		-----	
311	D7184	1.8		-0.79	
317	D4629	2.7		1.66	
322	D6069	2.7		1.66	
323		-----		-----	
334		-----		-----	
336		-----		-----	
347	D4629	2.8		1.93	
357	D4629	2.3		0.57	
402	D4629	1.68		-1.12	
444	D4629	2.73		1.74	
445	D4629	2.4		0.84	
453		-----		-----	
551		-----		-----	
555		-----		-----	
663		-----		-----	
823	D6069	1.79		-0.82	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
865		-----		-----	
866		-----		-----	
868	D4629	1.8		-0.79	
870		-----		-----	
912		-----		-----	
913		-----		-----	
963		-----		-----	
1011		-----		-----	
1040	D6069	1.965		-0.34	
1041	D6069	2.38		0.79	
1067	D6069	2.1		0.02	
1081	D4629	2.11		0.05	
1117	D7184	1.90		-0.52	
1151		-----		-----	
1201	D4629	1.8		-0.79	
1261		-----		-----	
1264	D7184	1.82		-0.74	
1291		-----		-----	
1294		-----		-----	
1307		-----		-----	
1319	D4629	2.2		0.30	
1357	D4629	1.66		-1.18	
1429	D4629	1.6		-1.34	
1538	D7184	2.1		0.02	
1728		-----		-----	
1741	D4629	1.90		-0.52	
1781		-----		-----	
1790	D6069	2.56		1.28	
1812		-----		-----	
1823	D6069	2.45		0.98	
1846	D4629	2.52		1.17	
1866	D7184	1.7		-1.07	
1880	D6069	1.65		-1.20	
7009		-----		-----	
9008	D6069	1.8		-0.79	
	normality	OK			
	n	31			
	outliers	0	Spike		
	mean (n)	2.091	2.03		Recovery < 103%
	st.dev. (n)	0.3656			
	R(calc.)	1.024			
	R(D4629:12)	1.027			

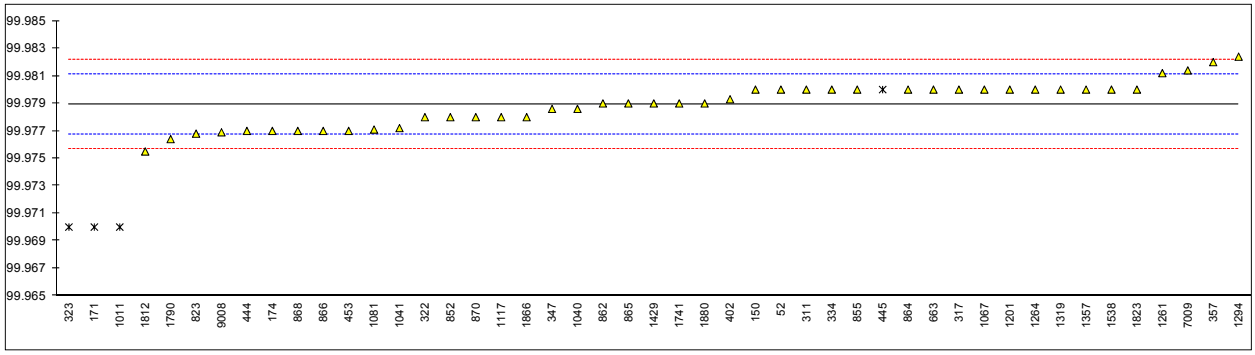

3.5
3
2.5
2
1.5
1
0.5
0
1429
1880
1357
402
1866
823
868
311
1201
9008
1264
171
1117
1741
1040
52
150
1067
1538
1081
1319
357
1041
445
1823
1846
1790
322
317
444
347

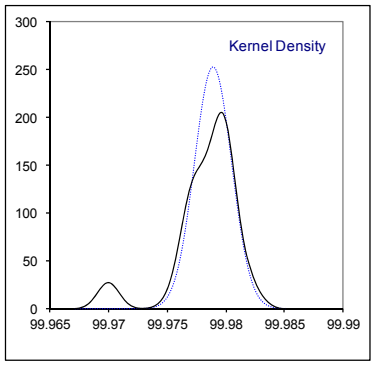

Kernel Density
1.2
1
0.8
0.6
0.4
0.2
0
0
1
2
3
4

Determination of Purity on Benzene sample #17020; results in %M/M

lab	method	value	mark	z(targ)	remarks
52	D7504	99.98		1.00	
150	D4492	99.98		1.00	
171	D4492	99.97	R(0.01)	-8.20	
174	D4492	99.977		-1.76	
311	D4492	99.98		1.00	
317	D4492	99.98		1.00	
322	D4492	99.978		-0.84	
323	D4492	99.97	R(0.01)	-8.20	
334	D4492	99.98		1.00	
336		-----		-----	
347	D4492	99.9786		-0.29	
357	D4492	99.982		2.84	
402	D4492	99.9793		0.36	
444	D4492	99.977		-1.76	
445	D4492	99.98	ex	1.00	Result excluded: reported result of Nonaromatic is a false negative
453	D4492	99.977		-1.76	
551		-----		-----	
555		-----		-----	
663	D4492	99.980	C	1.00	First reported 99.990
823	D4492	99.9768		-1.94	
852	D4492	99.978		-0.84	
855	D4492	99.980		1.00	
862	D4492	99.979		0.08	
864	D4492	99.980		1.00	
865	D4492	99.979		0.08	
866	D4492	99.977		-1.76	
868	D4492	99.977		-1.76	
870	D4492	99.978		-0.84	
912		-----		-----	
913		-----		-----	
963		-----		-----	
1011	D7360	99.97	R(0.01)	-8.20	
1040	D4492	99.9786		-0.29	
1041	D4492	99.9772		-1.58	
1067	In house	99.98		1.00	
1081	In house	99.9771		-1.67	
1117	D4492	99.978	C	-0.84	First reported 99.971
1151		-----		-----	
1201	D4492	99.98		1.00	
1261	D4492	99.9812		2.11	
1264	D4492	99.98		1.00	
1291		-----		-----	
1294		99.9824		3.21	
1307		-----		-----	
1319	D4492	99.98		1.00	
1357	D4492	99.98		1.00	
1429	D4492	99.979		0.08	
1538	D4492	99.98		1.00	
1728		-----		-----	
1741	D7504	99.979		0.08	
1781		-----		-----	
1790	In house	99.9764		-2.31	
1812		99.9755		-3.14	
1823	D4492	99.98		1.00	
1846		-----		-----	
1866	D4492	99.978		-0.84	
1880	D4492	99.979		0.08	
7009	D4492&D7504	99.9814		2.29	
9008	D4492	99.9769		-1.85	

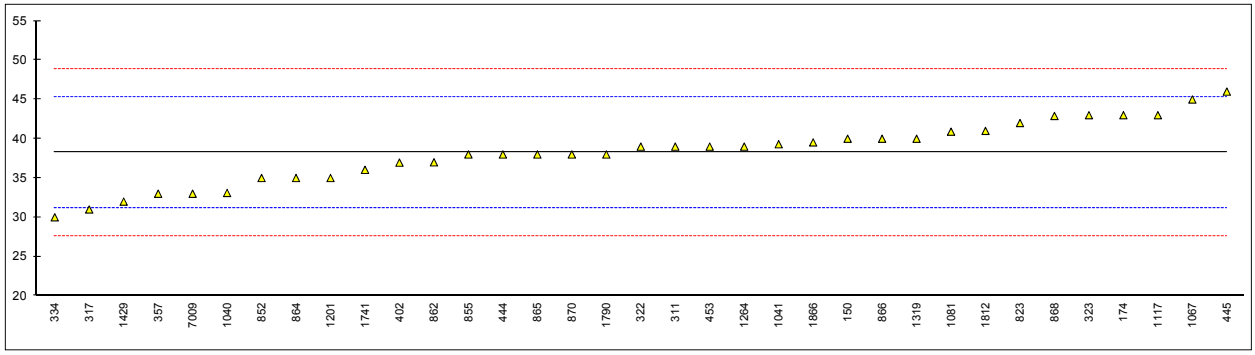
normality	OK
n	43
outliers	3 (+1 ex)
mean (n)	99.9789
st.dev. (n)	0.00159
R(calc.)	0.0045
R(D4492:10)	0.0030

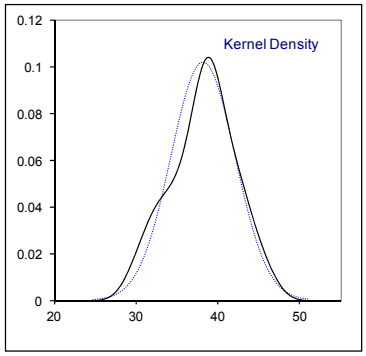

99.985
99.983
99.981
99.979
99.977
99.975
99.973
99.971
99.969
99.967
99.965
323 171 1011 1812 1790 823 9008 444 174 868 866 453 1081 1041 322 852 870 1117 1866 347 1040 862 865 1429 1741 1880 402 150 52 311 334 855 445 864 663 317 1067 1201 1264 1319 1357 1538 1823 1261 7009 357 1294


Kernel Density
300
250
200
150
100
50
0
99.965 99.97 99.975 99.98 99.985 99.99

Determination of Methylcyclohexane on Benzene sample #17020 in mg/kg

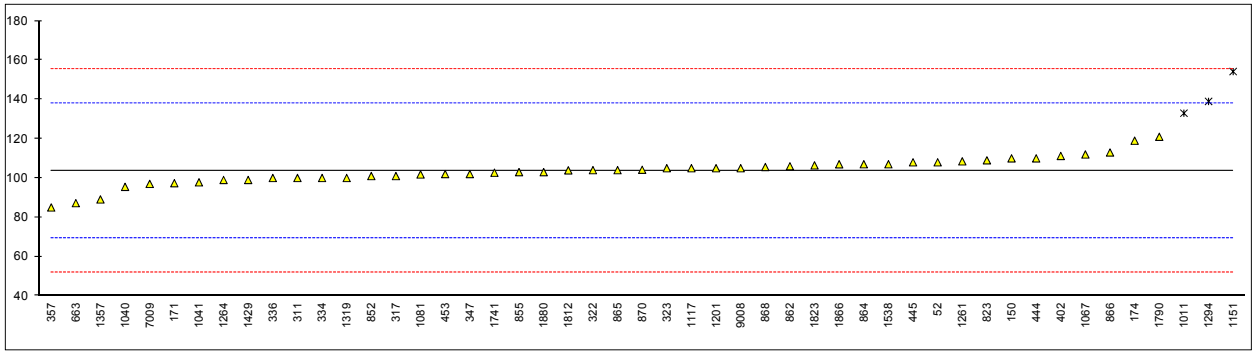
lab	method	value	mark	z(targ)	Remarks
52		-----		-----	
150		40		0.49	
171		-----		-----	
174	D4492	43		1.34	
311	D5713	39		0.21	
317	D5713	31		-2.05	
322	D4492	39		0.21	
323	D4492	43		1.34	
334	D4492	30	C	-2.33	First reported 0.003 mg/kg
336		-----		-----	
347		-----		-----	
357	D4492	33		-1.48	
402	D4492	36.96		-0.36	
444	D4492	38		-0.07	
445	D4492	46		2.19	
453	D4492	39		0.21	
551		-----		-----	
555		-----		-----	
663		-----		-----	
823	D5713	42		1.06	
852	D4492	35		-0.92	
855	D4492	38		-0.07	
862	D4492	37		-0.35	
864	D4492	35		-0.92	
865	D4492	38		-0.07	
866	D5713	40		0.49	
868	D4492	42.9		1.32	
870	D4492	38.0		-0.07	
912		-----		-----	
913		-----		-----	
963		-----		-----	
1011		-----		-----	
1040	D4492	33.1		-1.46	
1041	In house	39.3		0.30	
1067	In house	45	C	1.91	First reported 55
1081	INH-5713	40.9		0.75	
1117	D4492	43		1.34	
1151		-----		-----	
1201	D4492	35		-0.92	
1261		-----		-----	
1264	D4492	39		0.21	
1291		-----		-----	
1294		-----		-----	
1307		-----		-----	
1319	D4492	40		0.49	
1357		-----		-----	
1429	D4492	32		-1.77	
1538		-----		-----	
1728		-----		-----	
1741	D5713	36.045		-0.62	
1781		-----		-----	
1790	In house	38		-0.07	
1812		41		0.78	
1823		-----		-----	
1846		-----		-----	
1866	D4492	39.536		0.36	
1880		-----		-----	
7009	D4492&D7504	33		-1.48	
9008		-----		-----	
	normality	OK			
	n	35	Spike		
	outliers	0	30.97		Recovery < 124%
	mean (n)	38.25			
	st.dev. (n)	3.908			
	R(calc.)	10.94			
	R(Horwitz)	9.90			Compare R(D5713:14) = 3.72


55
50
45
40
35
30
25
20
334
317
1429
357
7009
1040
852
864
1201
1741
402
862
855
444
865
870
1790
322
311
453
1284
1041
1866
150
866
1319
1081
1812
823
868
323
174
1117
1067
445


Kernel Density
0.12
0.1
0.08
0.06
0.04
0.02
0
20
30
40
50

Determination of Toluene on Benzene sample #17020; results in mg/kg

lab	method	value	mark	z(targ)	Remarks
52	D7504	108		0.25	
150	D4492	110		0.37	
171	D4492	97.37		-0.36	
174	D4492	119		0.89	
311	D4492	100		-0.21	
317	D4492	101		-0.15	
322	D4492	104		0.02	
323	D4492	105		0.08	
334	D4492	100	C	-0.21	First reported 0.010 mg/kg
336	D4492	100	C	-0.21	First reported 0.01 mg/kg
347	D4492	102		-0.10	
357	D4492	85		-1.08	
402	D4492	111.23		0.44	
444	D4492	110		0.37	
445	D4492	108		0.25	
453	D4492	102		-0.10	
551		-----		-----	
555		-----		-----	
663	D4492	87.2	C	-0.96	First reported 50
823	D4492	109		0.31	
852	D4492	101		-0.15	
855	D4492	103		-0.04	
862	D4492	106		0.14	
864	D4492	107		0.19	
865	D4492	104		0.02	
866	D4492	113		0.54	
868	D4492	105.6		0.11	
870	D4492	104.2		0.03	
912		-----		-----	
913		-----		-----	
963		-----		-----	
1011	D7360	133	R(0.01)	1.70	
1040	D4492	95.5		-0.47	
1041	D4492	97.8		-0.34	
1067	In house	112		0.48	
1081	In house	101.8		-0.11	
1117	D4492	105		0.08	
1151	In house	154.21	R(0.01)	2.93	
1201	D4492	105		0.08	
1261	D4492	108.5		0.28	
1264	D4492	99		-0.27	
1291		-----		-----	
1294		139	C,R(0.01)	2.05	Reported 0.0139 mg/kg
1307		-----		-----	
1319	D4492	100		-0.21	
1357	D4492	89.1		-0.84	
1429	D4492	99		-0.27	
1538	D4492	107		0.19	
1728		-----		-----	
1741	D7504	102.70		-0.06	
1781		-----		-----	
1790	In house	121		1.01	
1812		103.9		0.01	
1823	D4492	106.43		0.16	
1846		-----		-----	
1866	D4492	106.991		0.19	
1880	D4492	103		-0.04	
7009	D4492&D7504	97		-0.39	
9008	D4492	105		0.08	
	normality	suspect			
	n	46			
	outliers	3	Spike		
	mean (n)	103.66	100.32		Recovery <103%
	st.dev. (n)	6.857			
	R(calc.)	19.20			
	R(D4492:10)	48.26			


180
160
140
120
100
80
60
40
357
663
1357
1040
7009
171
1041
1264
1429
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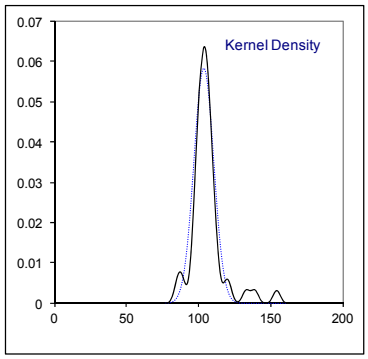
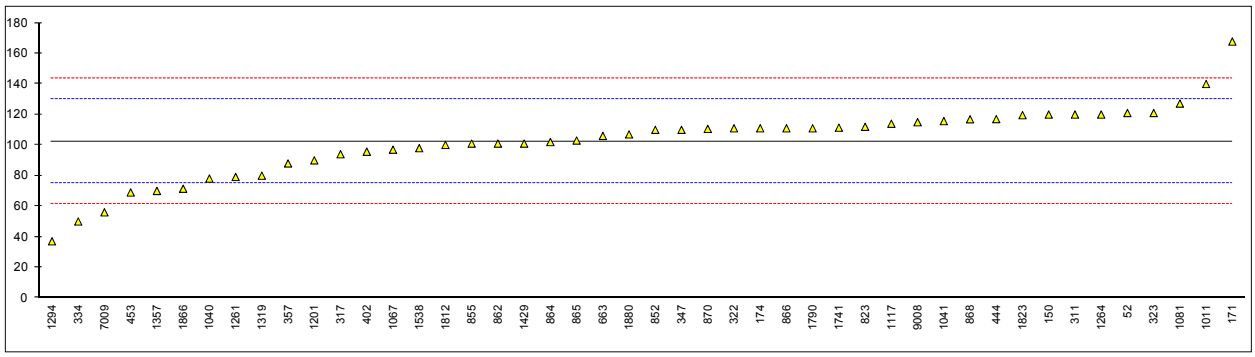
311
334
1319
852
317
1081
453
347
1741
855
1880
1812
322
865
870
323
1117
1201
9008
868
862
1823
1866
864
1538
445
52
1261
823
150
444
402
1067
866
174
1790
1011
1294
1151


Kernel Density
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
50
100
150
200

Determination of Nonaromatics on Benzene sample #17020; results in mg/kg

lab	method	value	mark	z(targ)	Remarks
52	D7504	121		1.36	
150	D4492	120		1.29	
171	D4492	167.80		4.77	
174	D4492	111		0.63	
311	D4492	120		1.29	
317	D4492	94		-0.61	
322	D4492	111		0.63	
323	D4492	121		1.36	
334	D4492	50	C	-3.81	First reported 0.005 mg/kg
336	D4492	<500	C	-----	First reported <0.05 mg/kg
347	D4492	110		0.56	
357	D4492	88		-1.04	
402	D4492	95.67		-0.49	
444	D4492	117		1.07	
445	D4492	<10		<6.73	False negative test result?
453	D4492	69		-2.43	
551		-----		-----	
555		-----		-----	
663	D4492	106	C	0.27	First reported 50
823	D4492	112		0.70	
852	D4492	110		0.56	
855	D4492	101		-0.10	
862	D4492	101		-0.10	
864	D4492	102		-0.02	
865	D4492	103		0.05	
866	D4492	111		0.63	
868	D4492	116.9		1.06	
870	D4492	110.6		0.60	
912		-----		-----	
913		-----		-----	
963		-----		-----	
1011	D7360	140		2.74	
1040	D4492	78.1		-1.77	
1041	D4492	115.7		0.97	
1067	In house	97		-0.39	
1081	In house	127.2		1.81	
1117	D4492	114		0.85	
1151		-----		-----	
1201	D4492	90		-0.90	
1261	D4492	79.12		-1.69	
1264	D4492	120		1.29	
1291		-----		-----	
1294		37	C	-4.76	Reported 0.0037
1307		-----		-----	
1319	D4492	80		-1.63	
1357	D4492	70		-2.36	
1429	D4492	101		-0.10	
1538	D4492	98		-0.32	
1728		-----		-----	
1741	D7504	111.40		0.66	
1781		-----		-----	
1790	In house	111		0.63	
1812		100.1		-0.16	
1823	D4492	119.60		1.26	
1846		-----		-----	
1866	D4492	71.432		-2.25	
1880	D4492	107		0.34	
7009	D4492&D7504	56		-3.38	
9008	D4492	115		0.92	

normality	suspect
n	46
outliers	0
mean (n)	102.34
st.dev. (n)	23.225
R(calc.)	65.03
R(D4492:10)	38.43


180
160
140
120
100
80
60
40
20
0
1294
334
7009
453
1357
1866
1040
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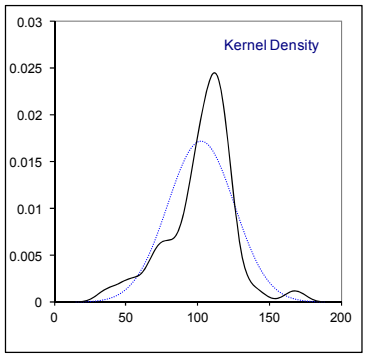
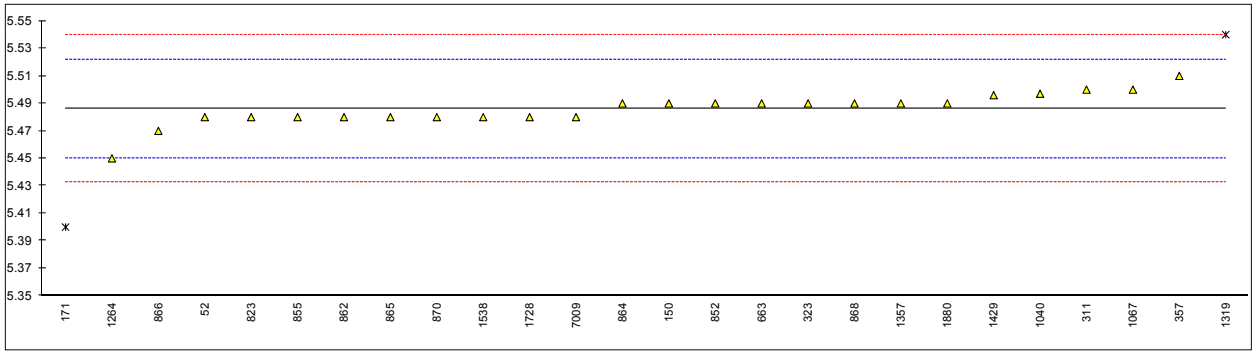
1319
357
1201
317
402
1067
1538
1812
855
862
1429
864
865
663
1880
852
347
870
322
174
866
1790
1741
823
1117
9008
1041
868
444
1823
150
311
1264
52
323
1081
1011
171

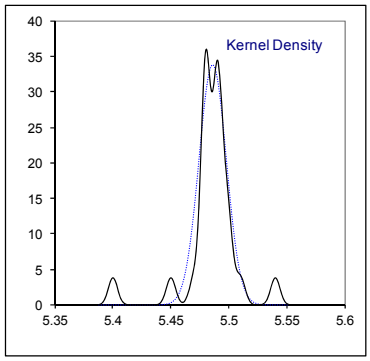

Kernel Density
0.03
0.025
0.02
0.015
0.01
0.005
0
0
50
100
150
200

Determination of Solidification Point (anhydrous) on Benzene sample #17020; results in °C

lab	method	value	mark	z(targ)	remarks
52	D852	5.48		-0.33	
150	D852	5.49		0.23	
171	D852	5.40	R(0.01)	-4.81	
174		-----		-----	
311	D852	5.50		0.79	
317		-----		-----	
322		-----		-----	
323	D852	5.49		0.23	
334		-----		-----	
336		-----		-----	
347		-----		-----	
357	D852	5.51		1.35	
402		-----		-----	
444		-----		-----	
445		-----		-----	
453		-----		-----	
551		-----		-----	
555		-----		-----	
663	D852	5.49		0.23	
823	D852	5.48		-0.33	
852	D852	5.49		0.23	
855	D852	5.48		-0.33	
862	D852	5.48		-0.33	
864	D852	5.49		0.23	
865	D852	5.48		-0.33	
866	D852	5.47		-0.89	
868	D852	5.49		0.23	
870	D852	5.48		-0.33	
912		-----		-----	
913		-----		-----	
963		-----		-----	
1011		-----		-----	
1040	DIN51798	5.497		0.62	
1041		-----		-----	
1067	D852	5.50		0.79	
1081		-----		-----	
1117		-----		-----	
1151		-----		-----	
1201		-----		-----	
1261		-----		-----	
1264	D852	5.45		-2.01	
1291		-----		-----	
1294		-----		-----	
1307		-----		-----	
1319	D852	5.54	R(0.01)	3.03	
1357	D852	5.49	C	0.23	First reported 5.39
1429	D852	5.496		0.56	
1538	D852	5.48		-0.33	
1728	D852	5.48		-0.33	
1741		-----		-----	
1781		-----		-----	
1790		-----		-----	
1812		-----		-----	
1823		-----		-----	
1846		-----		-----	
1866		-----		-----	
1880	D852	5.49		0.23	
7009	D852	5		-0.33	
9008		-----		-----	

normality	not OK
n	24
outliers	2
mean (n)	5.486
st.dev. (n)	0.0118
R(calc.)	0.033
R(D852:16)	0.05


5.55
5.53
5.51
5.49
5.47
5.45
5.43
5.41
5.39
5.37
5.35
171
1264
866
52
823
855
862
865
870
1538
1728
7009
864
150
852
663
323
868
1357
1880
1429
1040
311
1067
357
1319


Kernel Density
40
35
30
25
20
15
10
5
0
5.35
5.4
5.45
5.5
5.55
5.6

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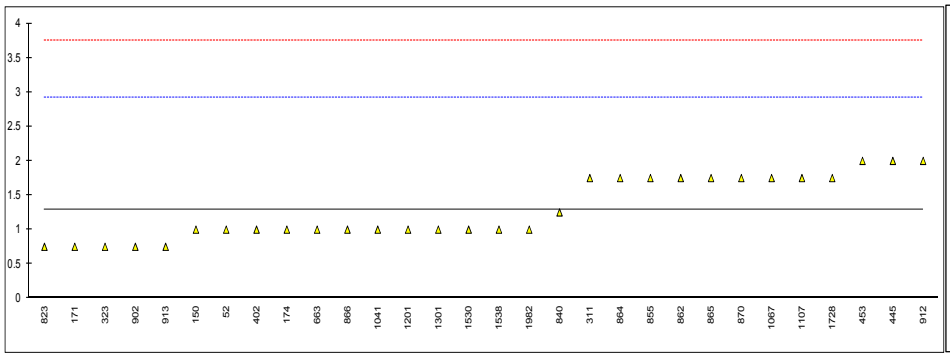
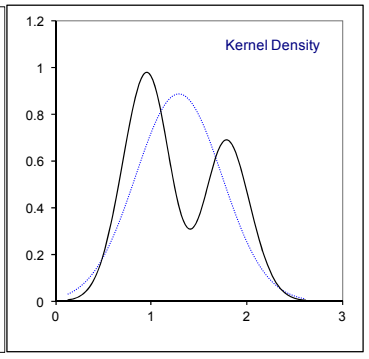
Determination of Acid Wash Color (acid layer) on Toluene sample #17021

lab	method	value	mark	z(targ)	remarks
52	D848	1		-0.38	
150	D848	1		-0.38	
171	D848	1-		-0.69	
174	D848	1		-0.38	
311	D848	2-		0.53	
323	D848	-1		-0.69	
334		-----		-----	
343	D848	2	C	0.83	First reported PASS
402	D848	1		-0.38	
445	D848	2		0.83	
453	D848	2		0.83	
551		-----		-----	
555		-----		-----	
663	D848	1		-0.38	
823	D848	1-		-0.69	
840	D848	1+		-0.08	
855	D848	No.2-		0.53	
862	D848	NO.2-		0.53	
864	D848	No.2-		0.53	
865	D848	No.2-		0.53	
866	D848	No.1		-0.38	
870	D848	No.2-		0.53	
902	D848	1-		-0.69	
912	D848	2		0.83	
913	D848	less than 1.0		-0.69	
1011		-----		-----	
1040		-----		-----	
1041	D848	1		-0.38	
1067	D848	2-		0.53	
1107	D848	2-		0.53	
1151		-----		-----	
1201	D848	1		-0.38	
1291		-----		-----	
1301	D848	1		-0.38	
1307		-----		-----	
1530	D848	1		-0.38	
1538	D848	1		-0.38	
1728	D848	2-		0.53	
1812		-----		-----	
1982	D848	1		-0.38	
7002		-----		-----	

normality	OK
n	31
outliers	0
mean (n)	1.31 (1+)
st.dev. (n)	0.461
R(calc.)	1.29
R(D848:14)	2.30

*) In the calculation of the mean, standard deviation, reproducibility and in the graphs, a reported value of ‘y-‘ or ‘less than y’ is changed into y-0.25 (for example 1- into 0.75) and ‘y+’ is changed into y+0.25 (for example 1+ into 1.25).





Determination of Appearance on Toluene sample #17021

lab	method	value	mark	z(targ)	remarks
52	D4176	Pass		-----	
150	E2680	Pass		-----	
171	E2680	Pass		-----	
174	E2680	CFSM		-----	
311	INH-402	bright & clear		-----	
323	D4176	C&B		-----	
334		-----		-----	
343	E2680	PASS		-----	
402		-----		-----	
445	E2680	Pass		-----	
453	Visual	Clear & Bright		-----	
551		-----		-----	
555		-----		-----	
663	Visual	B&C		-----	
823	E2680	Pass		-----	
840	E2680	Pass		-----	
855	E2680	Pass		-----	
862	E2680	Pass		-----	
864	Visual	Pass		-----	
865		Pass		-----	
866	E2680	Pass		-----	
870	E2680	Pass		-----	
902	E2680	PASS		-----	
912	E2680	Pass		-----	
913	E2680	Clear		-----	
1011		-----		-----	
1040		-----		-----	
1041		-----		-----	
1067	E2680	Pass		-----	
1107		-----		-----	
1151		-----		-----	
1201	D4176	Bright and clear		-----	
1291		-----		-----	
1301	Visual	CBFSM		-----	Reported: Clear & bright,free from suspended matter
1307		-----		-----	
1530		-----		-----	
1538	Visual	c&b		-----	
1728	Visual	CLEAR		-----	
1812		-----		-----	
1982	Visual	colourless		-----	
7002		pass		-----	
	normality	unknown			
	n	28			
	outliers	n.a.			
	mean (n)	Pass			
	st.dev. (n)	n.a.			
	R(calc.)	n.a.			
	R(E2680:09)	n.a.			

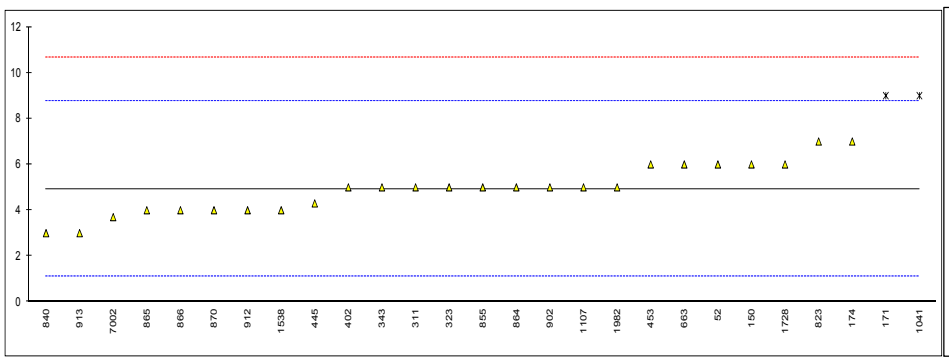
Abbreviations:
C&B / B&C = clear and bright / bright and clear
CFSM = clear and free from suspended matter
CBFSM = clear& bright and free from suspended matter

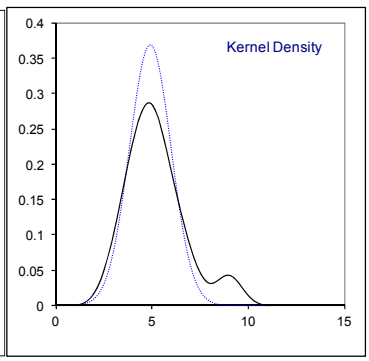
Determination of Color (Pt-Co scale) on Toluene sample #17021

lab	method	value	mark	z(targ)	remarks
52	D5386	6		0.56	
150	D5386	6		0.56	
171	D5386	9	R(0.05)	2.13	
174	D5386	7		1.09	
311	D1209	5		0.04	
323	D5386	5		0.04	
334		-----		-----	
343	D5386	5		0.04	
402	D1209	5		0.04	
445	D1209	4.3		-0.32	
453	D1209	6		0.56	
551		-----		-----	
555		-----		-----	
663	D5386	6		0.56	
823	D5386	7		1.09	
840	D1209	3		-1.00	
855	D5386	5		0.04	
862	D1209	<5		-----	
864	D5386	5		0.04	
865	D5386	4		-0.48	
866	D1209	4		-0.48	
870	D1209	4		-0.48	
902	D5386	5		0.04	
912	D5386	4		-0.48	
913	D5386	3		-1.00	
1011		-----		-----	
1040	ISO6271	< 5		-----	
1041	ISO6271	9	R(0.05)	2.13	
1067	D1209	< 5		-----	
1107	D1209	5		0.04	
1151		-----		-----	
1201	D1209	<5		-----	
1291		-----		-----	
1301	D1209	LT5		-----	
1307		-----		-----	
1530	D5386	<3		-----	
1538	D1209	4		-0.48	
1728	D1209	6		0.56	
1812		-----		-----	
1982	ISO6271	5		0.04	
7002		3.7		-0.64	

	normality	OK
	n	25
	outliers	2
	mean (n)	4.92
	st.dev. (n)	1.081
	R(calc.)	3.03
	R(D5386:16)	5.36

Compare R(D1209) = 7





Determination of Copper Corrosion on Toluene sample #17021

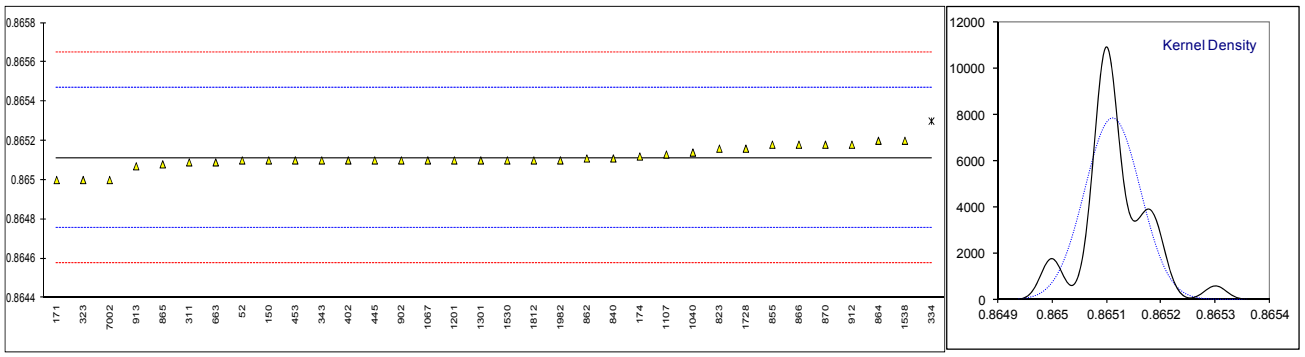
lab	method	value	mark	z(targ)	remarks
52	D849	1a		-----	
150	D849	1a		-----	
171	D849	1a		-----	
174		-----		-----	
311	D849	1		-----	
323	D849	CuCor1A		-----	
334	D849	pass		-----	
343	D849	1A		-----	
402		-----		-----	
445	D849	1A		-----	
453		-----		-----	
551		-----		-----	
555		-----		-----	
663	D849	1a		-----	
823	D849	1a		-----	
840	D849	1A		-----	
855	D849	1a		-----	
862	D849	1a		-----	
864	D849	1a		-----	
865		1a		-----	
866	D849	1a		-----	
870	D849	1a		-----	
902		-----		-----	
912	D849	1a		-----	
913	D849	1a		-----	
1011		-----		-----	
1040		-----		-----	
1041		-----		-----	
1067	D849	1A		-----	
1107	D849	1		-----	
1151		-----		-----	
1201	D849	1A		-----	
1291		-----		-----	
1301	D849	1A		-----	
1307		-----		-----	
1530		-----		-----	
1538		-----		-----	
1728	D849	1A		-----	
1812		-----		-----	
1982		-----		-----	
7002		-----		-----	

normality	unknown
n	24
outliers	n.a.
mean (n)	1a
st.dev. (n)	n.a.
R(calc.)	n.a.
R(D849:15)	n.a.

Determination of Density at 20°C on Toluene sample #17021: results in kg/L

lab	method	value	mark	z(targ)	remarks
52	D4052	0.8651		-0.06	
150	D4052	0.8651		-0.06	
171	D4052	0.8650		-0.62	
174	D4052	0.86512		0.05	
311	D4052	0.86509		-0.12	
323	D4052	0.8650		-0.62	
334	ISO12185	0.8653	C,R(0.05)	1.06	First reported 0.8563
343	ISO12185	0.8651		-0.06	
402	D4052	0.8651		-0.06	
445	D4052	0.8651		-0.06	
453	ISO12185	0.8651	C	-0.06	Reported 865.1
551		-----		-----	
555		-----		-----	
663	D4052	0.86509		-0.12	
823	ISO12185	0.86516		0.27	
840	D4052	0.86511		-0.01	
855	D4052	0.86518		0.38	
862	D4052	0.86511		-0.01	
864	D4052	0.86520		0.50	
865	ISO12185	0.86508		-0.18	
866	D4052	0.86518		0.38	
870	D4052	0.86518		0.38	
902	D4052	0.8651		-0.06	
912	D4052	0.86518		0.38	
913	D4052	0.86507		-0.23	
1011		-----		-----	
1040	ISO12185	0.86514	C	0.16	Reported 865.14
1041		-----		-----	
1067	D4052	0.8651		-0.06	
1107	D4052	0.86513		0.10	
1151		-----		-----	
1201	D4052	0.8651		-0.06	
1291		-----		-----	
1301	D4052	0.8651		-0.06	
1307		-----		-----	
1530	ISO12185	0.8651		-0.06	
1538	ISO3675	0.8652	C	0.50	First reported 0.866
1728	ISO12185	0.86516		0.27	
1812	ISO12185	0.8651		-0.06	
1982	ISO12185	0.8651		-0.06	
7002		0.8650		-0.62	

normality	OK
n	33
outliers	1
mean (n)	0.86511
st.dev. (n)	0.000051
R(calc.)	0.00014
R(ISO12185:96)	0.0005



Determination of Distillation on Toluene sample #17021; results in °C

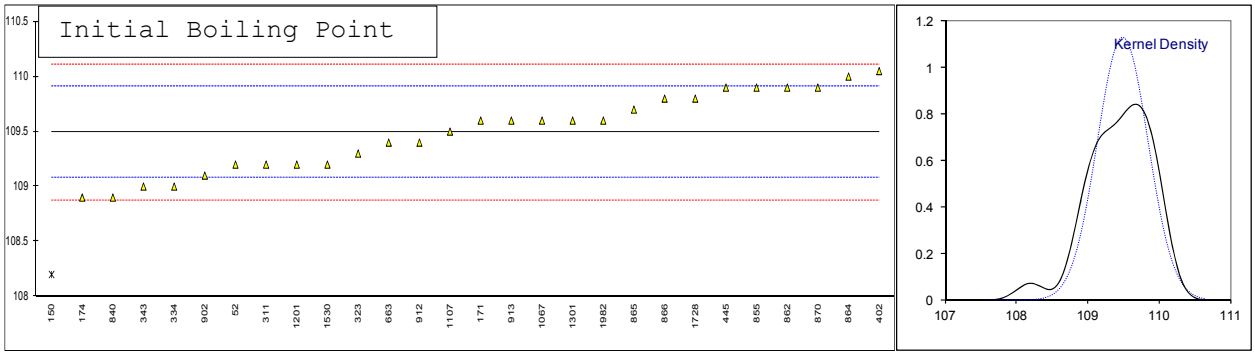
lab	method	mode	IBP	mark	z(targ)	50%	mark	z(targ)	DP	mark	z(targ)
52	D850	Automated	109.2		-1.40	110.6		-0.18	111.8		-----
150	D850	Automated	108.2	C,R(0.05)	-6.22	110.6		-0.18	112.2		-----
171	D850	Automated	109.6		0.53	110.5		-1.97	113.7		-----
174	D1078	Automated	108.9		-2.85	110.6		-0.18	113.1		-----
311	D850	Automated	109.2		-1.40	110.6		-0.18	112.3		-----
323	D850	Manual	109.3		-0.92	110.7		1.62	-----		-----
334	D850	Automated	109.0	C	-2.36	112.1	C,R(0.01)	26.74	111.9		-----
343	D850	Automated	109.0		-2.36	110.6		-0.18	113.4		-----
402	D850	Manual	110.05		2.70	110.65		0.72	114.65		-----
445	D850	Manual	109.9		1.97	110.5		-1.97	113.1		-----
453			-----		-----	-----		-----	-----		-----
551			-----		-----	-----		-----	-----		-----
555			-----		-----	-----		-----	-----		-----
663	D850	Automated	109.4		-0.44	110.6		-0.18	115.4	C	-----
823			-----		-----	-----		-----	-----		-----
840	D850	Automated	108.9		-2.85	110.5		-1.97	112.5		-----
855	D850	Manual	109.9		1.97	110.7		1.62	114.5		-----
862	D850	Manual	109.9		1.97	110.6		-0.18	114.5		-----
864	D850		110.0		2.45	110.7		1.62	114.6		-----
865	D850	Manual	109.7		1.01	110.6		-0.18	114.6		-----
866	D850	Manual	109.8		1.49	110.7		1.62	114.6		-----
870	D850	Manual	109.9		1.97	110.7		1.62	114.5		-----
902	D850	Automated	109.1		-1.88	110.6		-0.18	113.0		-----
912	D850	Automated	109.4		-0.44	110.4	R(0.05)	-3.77	115.0		-----
913	D850	Manual	109.6		0.53	110.6		-0.18	114.6		-----
1011			-----		-----	-----		-----	-----		-----
1040			-----		-----	-----		-----	-----		-----
1041			-----		-----	-----		-----	-----		-----
1067	D850	Manual	109.6		0.53	110.6		-0.18	114.6		-----
1107	D850	Automated	109.5		0.04	110.6		-0.18	113.2		-----
1151			-----		-----	-----		-----	-----		-----
1201	D850	Automated	109.2		-1.40	110.6		-0.18	112.5		-----
1291			-----		-----	-----		-----	-----		-----
1301	D850		109.6		0.53	111.0	R(0.01)	7.00	114.0		-----
1307			-----		-----	-----		-----	-----		-----
1530	D850	Manual	109.2		-1.40	110.6		-0.18	114.0		-----
1538			-----		-----	-----		-----	-----		-----
1728	D850	Manual	109.8		1.49	110.6		-0.18	113.0	C	-----
1812			-----		-----	-----		-----	-----		-----
1982	D850	Automated	109.6		0.53	110.6		-0.18	113.4		-----
7002			-----		-----	-----		-----	-----		-----
	normality		OK			OK			OK		
	n		27			25			27		
	outliers		1			3			0		
	mean (n)		109.49			110.61			113.65		
	st.dev. (n)		0.354			0.058			1.031		
	R(calc.)		0.99			0.16			2.89		
	R(D850:16)	Automated	0.58			0.16			(0.46)	*)	

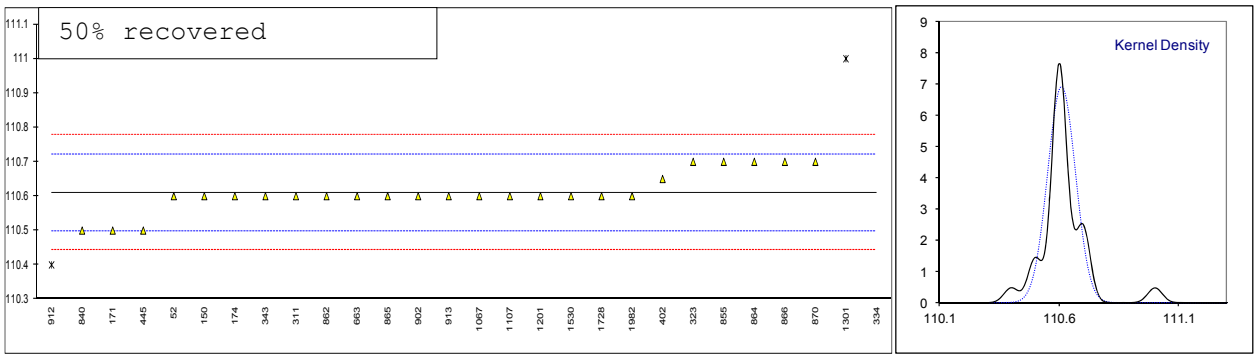
Compare R(D850:16) – Manual = 0.47

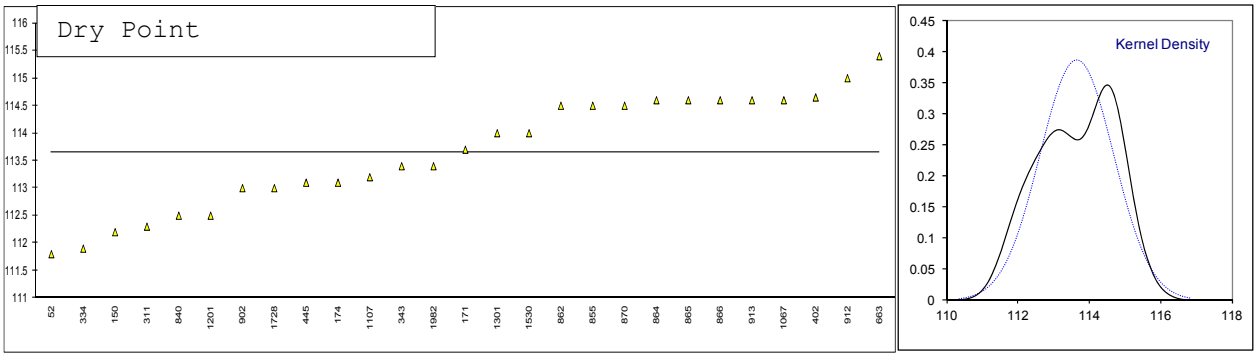
*) The reproducibility of the reference method is most likely not applicable for sample #17021 due to the higher level of impurities in this sample. (The average purity of sample #17021 is 98.443, with a calculated reproducibility of 0.441)

Lab 150: First reported IBP=108.6
Lab 334: First reported IBP=108.6, 50%=110.1
Lab 663: First reported DP=115.6
Lab 1728: First reported DP=110.8

Theoretical mid boiling point = 110.6 °C


Initial Boiling Point
Kernel Density

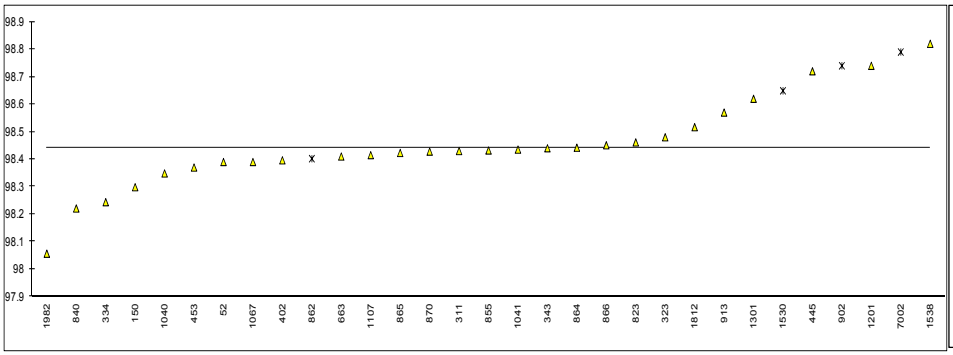

50% recovered
Kernel Density

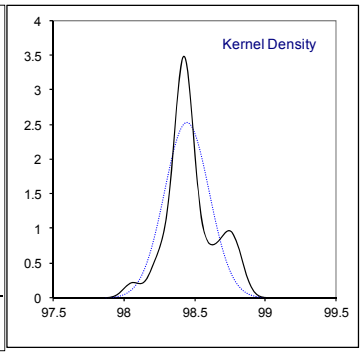

Dry Point
Kernel Density

Determination of Purity on Toluene sample #17021; results in %M/M

lab	method	value	mark	z(targ)	remarks
52	D7504	98.39		-----	
150	D7504	98.2985		-----	
171		-----		-----	
174		-----		-----	
311	D2360	98.43		-----	
323	D6526	98.48		-----	
334	D2360	98.244		-----	
343	D2360	98.44		-----	
402	D2360	98.39623		-----	
445	D6526	98.72		-----	
453	D2360	98.37		-----	
551		-----		-----	
555		-----		-----	
663	D6563	98.410		-----	
823	D2360	98.4613		-----	
840	D7504	98.221		-----	
855	D7504	98.432		-----	
862	D2360	98.402	ex	-----	Result excluded: no nonaromatics reported.
864	D7504	98.442		-----	
865		98.423		-----	
866	D2360	98.451		-----	
870	D2360	98.428		-----	
902	INH-135	98.74	C, ex	-----	Result excluded: no benzene and no nonaromatics reported. First reported 99.74
912		-----		-----	
913	D2360	98.57		-----	
1011		-----		-----	
1040	D6526	98.3485		-----	
1041	In house	98.4352		-----	
1067	In house	98.39		-----	
1107	D6526	98.415		-----	
1151		-----		-----	
1201	D2360	98.74		-----	
1291		-----		-----	
1301	D2360	98.62		-----	
1307		-----		-----	
1530		98.649	ex	-----	Result excluded: no nonaromatics reported.
1538	D2360	98.82		-----	
1728		-----		-----	
1812		98.5167		-----	
1982	D2360	98.0566		-----	
7002		98.79	ex	-----	Results excluded: no benzene and no nonaromatics reported.
	normality	suspect			
	n	27			
	outliers	0 (+4 ex)			
	mean (n)	98.4426			
	st.dev. (n)	0.15759			
	R(calc.)	0.4413			
	R(D7504:16)	(0.0129)	*)		

*) (R(D7504) is based on a purity level much higher than the purity level of sample #17021)

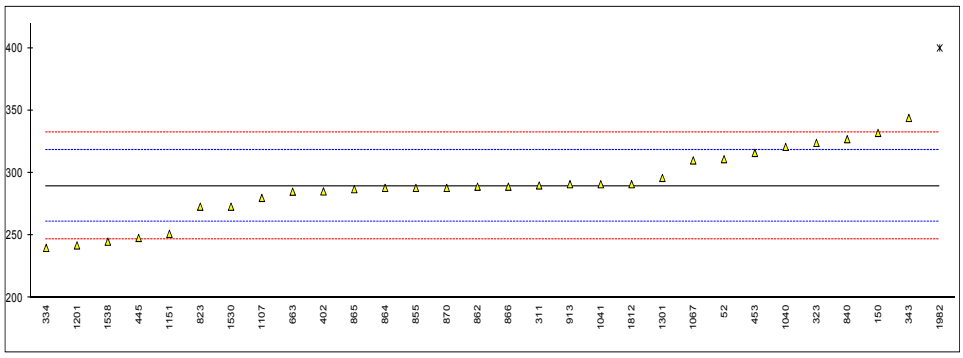


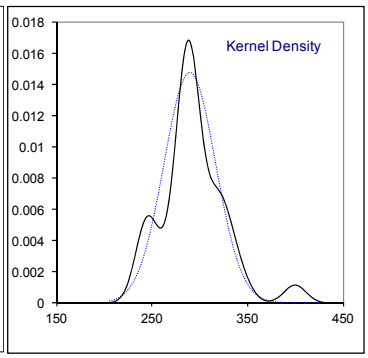


Determination of Benzene on Toluene sample #17021; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7504	311		1.50	
150	D7504	332		2.97	
171		-----		-----	
174		-----		-----	
311	D2360	290		0.04	
323	D6526	324		2.41	
334	D2360	240	C	-3.46	First reported 0.024
343	D2360	344	C	3.81	First reported 364
402	D2360	285.22		-0.30	
445	D6526	248		-2.90	
453	D2360	316		1.85	
551		-----		-----	
555		-----		-----	
663	D6563	285		-0.31	
823	D2360	273		-1.15	
840	D7504	327.0		2.62	
855	D7504	288		-0.10	
862	D2360	289		-0.03	
864	D7504	288		-0.10	
865		287		-0.17	
866	D2360	289		-0.03	
870	D2360	288		-0.10	
902		-----		-----	
912		-----		-----	
913	D2360	291		0.11	
1011		-----		-----	
1040	D6526	320.8		2.19	
1041	In house	291		0.11	
1067	In house	310		1.43	
1107	D6526	280		-0.66	
1151		251.26		-2.67	
1201	D2360	242		-3.32	
1291		-----		-----	
1301	D2360	296		0.45	
1307		-----		-----	
1530		273		-1.15	
1538	D2360	245		-3.11	
1728		-----		-----	
1812		291		0.11	
1982	D2360	400	C,R(0.05)	7.72	First reported 20.5
7002		-----		-----	

normality	OK
n	29
outliers	1
mean (n)	289.5
st.dev. (n)	27.09
R(calc.)	75.8
R(D7504:16)	40.1

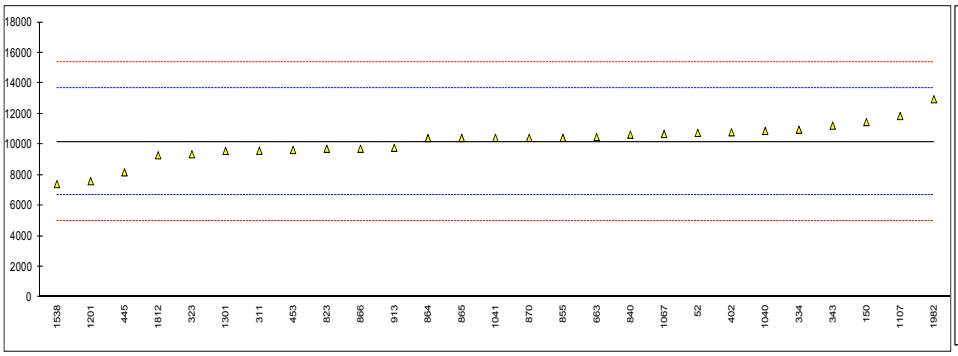


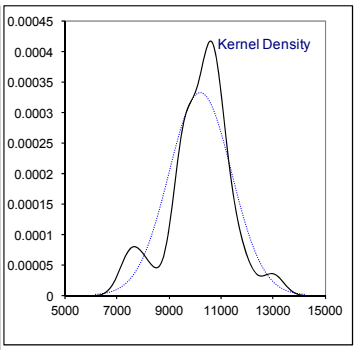


Determination of Nonaromatics on Toluene sample #17021; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7504	10766		0.34	
150	D7504	11471		0.74	
171		-----		-----	
174		-----		-----	
311	D2360	9590		-0.34	
323	D6526	9360		-0.47	
334	D2360	10970	C	0.45	First reported 1.097
343	D2360	11235		0.61	
402	D2360	10799.27		0.36	
445	D6526	8181		-1.15	
453	D2360	9646		-0.31	
551		-----		-----	
555		-----		-----	
663	D6563	10485	C	0.18	First reported 10.485
823	D2360	9720		-0.26	
840	D7504	10645.0		0.27	
855	D7504	10439		0.15	
862		-----		-----	
864	D7504	10423		0.14	
865		10426		0.14	
866	D2360	9724		-0.26	
870	D2360	10438		0.15	
902		-----		-----	
912		-----		-----	
913	D2360	9785	C	-0.23	First reported 0.865, reported 0.9785
1011		-----		-----	
1040	D6526	10888.5		0.41	
1041	In house	10437		0.15	
1067	In house	10690		0.29	
1107	D6526	11866		0.97	
1151		-----		-----	
1201	D2360	7600		-1.48	
1291		-----		-----	
1301	D2360	9578		-0.35	
1307		-----		-----	
1530		-----		-----	
1538	D2360	7410		-1.59	
1728		-----		-----	
1812		9299	C	-0.51	First reported 989.4
1982	D2360	12966.6		1.60	
7002		-----		-----	
	normality	suspect			
	n	27			
	outliers	0			
	mean (n)	10179.2			
	st.dev. (n)	1200.55			
	R(calc.)	3361.5			
	R(D2360:11)	4868.3 *)			Compare R(D7504) = 9200.4 *)

*) In the literature the reproducibility is given at a concentration level which is far below the concentration level of sample #17021

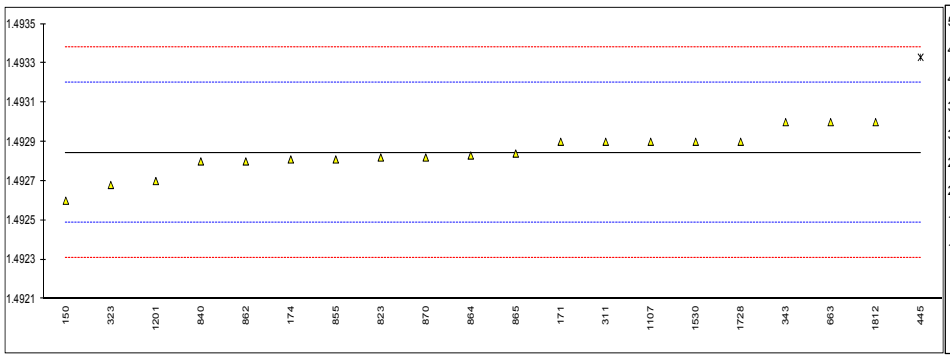


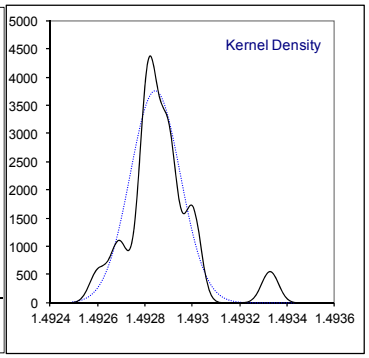


Determination of Refractive Index at 25 °C on Toluene sample #17021;

lab	method	value	mark	z(targ)	remarks
52		-----		-----	
150	D1218	1.4926	C	-1.36	First reported 1.4955
171	D1218	1.4929		0.32	
174	D1218	1.49281		-0.18	
311	D1218	1.4929		0.32	
323	D1218	1.49268		-0.91	
334		-----		-----	
343	D1218	1.4930		0.88	
402		-----		-----	
445	D1218	1.49333	G(0.01)	2.73	
453		-----		-----	
551		-----		-----	
555		-----		-----	
663	D1218	1.4930		0.88	
823	D1218	1.49282		-0.13	
840	D1218	1.4928		-0.24	
855	D1218	1.49281		-0.18	
862	D1218	1.49280		-0.24	
864	D1218	1.49283		-0.07	
865	D1218	1.49284		-0.02	
866		-----		-----	
870	D1218	1.49282		-0.13	
902		-----		-----	
912		-----		-----	
913		-----		-----	
1011		-----		-----	
1040		-----		-----	
1041		-----		-----	
1067		-----		-----	
1107	D1218	1.4929		0.32	
1151		-----		-----	
1201	D1218	1.4927		-0.80	
1291		-----		-----	
1301		-----		-----	
1307		-----		-----	
1530	D1218	1.4929		0.32	
1538		-----		-----	
1728		1.49290		0.32	
1812		1.4930		0.88	
1982		-----		-----	
7002		-----		-----	

normality	OK
n	19
outliers	1
mean (n)	1.49284
st.dev. (n)	0.000106
R(calc.)	0.00030
R(D1218:12)	0.0005





APPENDIX 2

Number of participants in the Benzene PT iis17C04

3 labs in	BELGIUM
3 labs in	BRAZIL
1 lab in	CANADA
9 labs in	CHINA, People's Republic
1 lab in	FINLAND
2 labs in	FRANCE
3 labs in	GERMANY
2 labs in	INDIA
1 lab in	IRAN, Islamic Republic of
1 lab in	JAPAN
2 labs in	KUWAIT
8 labs in	NETHERLANDS
1 lab in	OMAN
1 lab in	POLAND
1 lab in	PORTUGAL
2 labs in	ROMANIA
5 labs in	SAUDI ARABIA
1 lab in	SERBIA
1 lab in	SOUTH KOREA
1 lab in	SPAIN
1 lab in	TAIWAN
1 lab in	THAILAND
1 lab in	UNITED ARAB EMIRATES
4 labs in	UNITED KINGDOM
3 labs in	UNITED STATES OF AMERICA

Number of participants in the Toluene PT iis17C05

3 labs in	BELGIUM
3 labs in	BRAZIL
1 lab in	CANADA
6 labs in	CHINA, People's Republic
1 lab in	FRANCE
5 labs in	GERMANY
2 labs in	INDIA
1 lab in	IRAN, Islamic Republic of
3 labs in	NETHERLANDS
1 lab in	POLAND
1 lab in	PORTUGAL
2 labs in	ROMANIA
1 lab in	SAUDI ARABIA
1 lab in	SOUTH KOREA
1 lab in	SPAIN
1 lab in	THAILAND
1 lab in	TURKEY
1 lab in	UNITED ARAB EMIRATES
2 labs in	UNITED KINGDOM
3 labs in	UNITED STATES OF AMERICA
1 lab in	VIETNAM

APPENDIX 3

Abbreviations:

C	= final test result after checking of first reported suspect 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 outlier test
R(0.05)	= straggler in Rosner 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 calculations
n.a.	= not applicable
n.d.	= not detected
fr.	= first reported
SDS	= Safety Data Sheet

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