

Results of Proficiency Test
Benzene & Toluene
February 2015

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

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CONTENTS

1	INTRODUCTION.....	3
2	SET UP.....	3
2.1	ACCREDITATION.....	3
2.2	PROTOCOL.....	3
2.3	CONFIDENTIALITY STATEMENT.....	3
2.4	SAMPLES.....	4
2.5	STABILITY OF THE SAMPLES	5
2.6	ANALYSES.....	5
3	RESULTS.....	6
3.1	STATISTICS.....	6
3.2	GRAPHICS.....	7
3.3	Z-SCORES.....	7
4	EVALUATION.....	8
4.1	EVALUATION PER TEST	8
4.2	PERFORMANCE EVALUATION FOR THE GROUP OF LABORATORIES	12
4.3	COMPARISON OF THE PROFICIENCY TEST OF FEBRUARY 2015 WITH PREVIOUS PTs	13

Appendices:

1.	Data and statistical results	16
2.	Number of participants per country	55
3.	Abbreviations and literature	56

1 INTRODUCTION

Since 1999, the Institute for Interlaboratory Studies organizes proficiency tests for the analysis of Benzene and Toluene. In the annual proficiency testing program of 2014/2015, it was decided to continue the proficiency test for the analysis of Benzene and Toluene. In the interlaboratory study for Benzene 56 laboratories from 23 different countries have participated and for Toluene 40 participants in 23 countries have participated. See appendix 2 for the number of participants per country.

In this report, the results of the proficiency test Benzene and Toluene are presented and discussed. This report is also electronically available through the iis internet site www.iisnl.com.

2 SET UP

The Institute for Interlaboratory Studies (iis) in Spijkenisse, the Netherlands, was the organizer of this proficiency test. The analyses for fit-for-use and homogeneity determination were subcontracted to an accredited laboratory. It was decided to send one sample of Benzene (1 litre bottle, labelled #15013) and/or one sample of Toluene (1 litre bottle, labelled #15014) to the participants.

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 was the one as described for proficiency testing in the report 'iis Interlaboratory Studies: Protocol for the Organisation, Statistics and Evaluation' of April 2014 (iis-protocol, version 3.3). This protocol can be downloaded via the FAQ page of the iis website <http://www.iisnl.com>.

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 100 litre was spiked with 501.2 mg 1-Methyl-2-Pyrrolidinone (for the Nitrogen determination) and 242.6 mg o-Chlorotoluene (for the Organic Chlorides determination). The bulk sample was, after homogenisation, divided over 100 amber glass bottles of 1 litre, labelled #15013. The homogeneity of the subsamples #15013 was checked by determination of Density at 20°C in accordance with ASTM D4052 on 8 stratified randomly selected samples.

Benzene	Density at 20°C in kg/L
sample #15013-1	0.87895
sample #15013-2	0.87894
sample #15013-3	0.87895
sample #15013-4	0.87895
sample #15013-5	0.87895
sample #15013-6	0.87896
sample #15013-7	0.87896
sample #15013-8	0.87896

table 1: homogeneity test results of Benzene sub samples #15013

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

	Density at 20°C in kg/L
r (sample #15013)	0.00002
Target	ASTM 4052:02e1
0.3*R (target)	0.00015

table 2: evaluation of repeatabilities of subsamples #15013

The calculated repeatability for sample #15013 was in agreement with 0.3 times the corresponding target reproducibility. Therefore, homogeneity of the samples 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 60 brown glass bottles of 1 litre, labelled #15014. The homogeneity of the subsamples #15014 was checked by determination of Density at 20°C, according to ASTM D4052 on 8 stratified randomly selected samples.

Toluene	Density at 20°C in kg/L
sample #15014-1	0.86684
sample #15014-2	0.86684
sample #15014-3	0.86684
sample #15014-4	0.86683
sample #15014-5	0.86683
sample #15014-6	0.86684
sample #15014-7	0.86684
sample #15014-8	0.86684

table 3: homogeneity test results of Toluene sub samples #15014

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

	Density at 20°C in kg/L
r (sample #15014)	0.00001
Target	ASTM D4052:02e1
0.3*R (target)	0.00015

table 4: evaluation of repeatabilities of subsamples #15014

The calculated repeatability on Density for sample #15014 was in agreement with 0.3 times the corresponding target reproducibility. Therefore, homogeneity of the sub samples was assumed.

Depending on their registration to each of the participating laboratories one 1 litre bottle of Benzene labelled #15013 and/or one 1 litre bottle of Toluene labelled #15014 were sent on February 11, 2015.

2.5 STABILITY OF THE SAMPLES

The stability of Benzene and Toluene, 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 the Benzene sample #15013: Acid Wash Color, Acidity, Appearance, Bromine Index, Total Chloride, Organic Chlorides, Color Pt-Co, Density at 20°C, Distillation, Total Nitrogen, Purity, Methyl cyclohexane, Toluene, Non aromatics, and Solidification Point.

On Toluene sample #15014 were requested: Acid Wash Color, Appearance, Color Pt-Co, Copper Corrosion, Density at 20°C, Distillation, Purity, Benzene and Non aromatics.

To get comparable results a detailed report form, on which the units were prescribed as well as the required standards and a letter of instructions were prepared and made available on the data entry portal www.kpmd.co.uk/sgs-iis/. The detailed report form was also made available for download on the iis website www.iisnl.com.

3 RESULTS

During four weeks after sample despatch, the results of the individual laboratories were received. The original reported 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 fax was sent to those laboratories that had not yet reported any results at that moment.

Shortly after the deadline, the available results were screened for suspect data. A 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 results. Additional or corrected results are used for data analysis and original results are placed under 'Remarks' in the result tables in appendix 1.

3.1 STATISTICS

Statistical calculations were performed as described in the report 'iis Interlaboratory Studies: Protocol for the Organisation, Statistics and Evaluation' (iis-protocol, version 3.3) of April 2014.

For statistical evaluation the *unrounded* (when available) figures were used instead of the rounded results. 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. Not all data sets proved to have a normal distribution, in which cases the statistical evaluation of the results should be used with due care.

According to ISO 5725 the original 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 (ref. 16). 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 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 analysis results are plotted. The corresponding laboratory numbers are under 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 (see appendix 3; nos.14 and 15).

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 target standard deviation was calculated from the literature reproducibility by division with 2.8.

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:

$$Z_{(\text{target})} = (\text{result} - \text{average of PT}) / \text{target standard deviation}$$

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 proficiency test, problems were encountered during the execution. Laboratories in Brazil, India, Malaysia and Saudi Arabia did receive the samples late or not at all due to several reasons. For sample #15013 (Benzene) and #15014 (Toluene), respectively nine and three participants did not report any test results and respectively thirteen and ten laboratories reported the test results after the final reporting date.

Finally, for sample #15013 (Benzene) and sample #15014 (Toluene) in total 729 results were submitted. Observed were in total 15 outlying results, which is 2.1%. In proficiency studies, outlier percentages of 3% - 7.5% are normal.

4.1 EVALUATION PER SAMPLE AND TEST

In this section, the results are discussed per sample and test. The methods, which are 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. When no suitable test method is available, the Horwitz equation was used.

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.

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.

For Benzene sample #15013

Acid Wash Color: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in good agreement with the requirements of ASTM D848:14.

For the statistical analysis, the result expressed as y- or x+ were changed into numerical values as follows: y- changed into y-0.25 and x+ into x+0.25.

- Acidity: This determination was not problematic. The majority of laboratories report "no free acid" (NFA) or 0 mg NaOH/100 ml in accordance with ASTM D847:08.
- Appearance: No analytical problems were observed. All labs agreed about the appearance of the sample #15013, 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 Chloride: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D5194:13.
- Organic Chloride: This determination was not at all problematic. No statistical outliers were observed. The calculated reproducibility is in good agreement with the requirements of ASTM D5808:09a(2014).
The average recovery of Organic Chloride (theoretical increment of 0.78 mg/kg) may be good: "less than 100%" (the actual blank is unknown).
- Color Pt-Co: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in good agreement with the requirements of ASTM D1209:05e1(2011) and of ASTM D5886:10..
- Density at 20°C: This determination was not at all problematic. One statistical outlier was observed and one laboratory was excluded for measuring at a deviating temperature (15°C). However, the calculated reproducibility after rejection of the suspect data is in good agreement with the requirements of ASTM D4052:02e1. The current version of this method ASTM D4052:11 is only valid for gasolines, distillates, base stocks and lubricating oils. Therefore the reproducibility of this 2011 version may not be applicable for Benzene.
- Distillation: This determination was not problematic. No statistical outliers were observed. The calculated reproducibilities for Initial Boiling Point, 50% recovered and Dry Point are in good agreement with the requirements of ASTM D850:11.
From the reported results of the 50% recovered, it appears that one participant probably did not correct the results for barometric pressure and thermometer inaccuracy as described in ASTM D850 (paragraph 11).
- Total Nitrogen: This determination was not problematic. No statistical outliers were observed. One test result was excluded from the statistical evaluation as the reported test method was not equivalent to ASTM D6069. The calculated reproducibility after rejection of the suspect data is not in agreement with the requirements of ASTM D6069:01(2006). However, the

calculated reproducibility is in agreement with the less strict requirements of ASTM D4629:12.

The average recovery of Total Nitrogen (theoretical increment of 0.81 mg/kg) may be good: "less than 118%" (the actual blank is unknown).

Purity: This determination may not be problematic. No statistical outliers were observed. The calculated reproducibility is almost in agreement with the estimated reproducibility of ASTM D4492:10.

Methylcyclohexane: This determination may not be problematic. Twenty-four participants agreed on level of below 10 mg/kg, which is near or below the detection limit. The other four participants reported: 10, 36 and <50. It is remarkable that eighteen of the twenty-eight laboratories used ASTM D4492, a method which may be not applicable for the determination of methyl cyclohexane, while only six laboratories used ASTM D5713 a method that is suitable for the determination of methyl Cyclohexane in benzene.

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

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

Solidification Point: This determination may be problematic. No statistical outliers were observed. However the calculated reproducibility is almost in agreement with the requirements of ASTM D852:13.

For Toluene sample #15014

Acid Wash Color: This determination was not at all problematic. No statistical outliers were observed. The calculated reproducibility is in full agreement with the requirements of ASTM D848:14.

For the statistical analysis, the result expressed as y- or x+ were changed into numerical values as follows: y- changed into y-0.25 and x+ into x+0.25.

Appearance: No analytical problems were observed. All labs agreed about the appearance of the sample #15014, which was bright, clear and free of suspended matter (Pass).

Color Pt-Co: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in good agreement with the requirements of ASTM D1209:05e1(2011).

Copper Corrosion: No problems have been observed. All participants agreed on a result of 1 or 1A. One laboratory reported according to ISO2160, a method that is not equivalent to ASTM D849:11.

Density at 20°C: This determination was not problematic. Two statistical outliers were observed. However, the calculated reproducibility after rejection of the statistical outliers is in good agreement with the requirements of ASTM D4052:02e1. The current version of this method ASTM D4052:11 is valid only for gasolines, distillates, base stocks and lubricating oils. Therefore the reproducibility of this 2011 version may not be applicable for Toluene.

Distillation: This determination was not problematic for IBP and 50% recovered and may be problematic for DP. In total one statistical outlier was observed. The calculated reproducibilities for IBP and 50% recovered, after rejection of the statistical outlier, are in agreement with the requirements of ASTM D850:11. However, the calculated reproducibility for DP is almost in agreement with the requirements of ASTM D850:11. From the reported test results of the 50% recovered, it appears that one participant obviously did not correct the results for barometric pressure and thermometer inaccuracy as described in ASTM D850 (paragraph 11).

Purity: This determination was not problematic. Two statistical outliers were observed. However, the calculated reproducibility after rejection of the statistical outliers is in full agreement with the requirements of ASTM D2360:11.

Benzene: This determination may not be problematic at the concentration 52 mg/kg. Four statistical outliers were observed. However the calculated reproducibility after rejection of the statistical outliers is in full agreement with the estimated reproducibility limits calculated using the Horwitz equation.

Nonaromatics: This determination was not problematic. No statistical outlier were observed. The calculated reproducibility is in good agreement with the requirements of ASTM D2360:11.

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 standards) are compared in the next table.

Parameter	unit	n	average	2.8 *sd _R	R (lit)
Acid Wash Color		35	0.7 (1-)	1.0	2.1
Acidity	mg NaOH/100ml	35	NFA	n.a.	n.a.
Appearance		39	Pass	n.a.	n.a.
Bromine Index	mg Br/100g	33	2.3	2.7	4.6
Total Chloride	mg/kg	5	0.86	0.63	0.90
Organic Chlorides	mg/kg	18	0.79	0.42	1.30
Color Pt-Co		31	3.8	3.6	7.0
Density at 20°C	kg/l	41	0.8790	0.0002	0.0005
Distillation, IBP	°C	30	79.8	0.3	0.4
Distillation, 50%	°C	30	80.1	0.1	0.4
Distillation, DP	°C	29	80.2	0.2	0.4
Total Nitrogen	mg/kg	26	0.95	0.42	0.37
Purity	%M/M	40	99.991	0.005	0.004
Methylcyclohexane	mg/kg	24	<10	n.a.	n.a.
Toluene	mg/kg	37	10.0	2.9	4.3
Nonaromatics	mg/kg	41	71.5	41.5	33.6
Solidification Point	°C	25	5.49	0.06	0.05

Table 5: reproducibilities of Benzene sample #15013

Parameter	unit	n	average	2.8 *sd _R	R (lit)
Acid Wash Color		28	0.8 (1-)	0.6	2.1
Appearance		30	Pass	n.a.	n.a.
Color Pt-Co		24	3.8	4.5	7.0
Copper corrosion		25	1 (1A)	n.a.	n.a.
Density at 20°C	kg/L	34	0.8669	0.0002	0.0005
Distillation, IBP	°C	30	110.3	0.2	0.6
Distillation, 50% rec.	°C	29	110.6	0.1	0.2
Distillation, DP	°C	28	110.9	0.6	0.5
Purity	%M/M	32	99.961	0.015	0.021
Nonaromatics	mg/kg	27	52.1	7.3	12.9
Benzene	mg/kg	31	234.1	79.01	112.0

Table 6: reproducibilities of Toluene sample #15014

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 FEBRUARY 2015 WITH PREVIOUS PTS

	February 2015	February 2014	April 2013	April 2012
Number of reporting labs	51	58	41	46
Number of results reported	729	800	686	718
Statistical outliers	15	36	27	27
Percentage outliers	2.1%	4.5%	3.9%	3.8%

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 table:

	February 2015	February 2014	April 2013	April 2012
Acid Wash Color	++	n.e.	n.e.	n.e.
Acidity	n.e.	n.e.	n.e.	n.e.
Appearance	n.e.	n.e.	n.e.	n.e.
Bromine Index	+	+	+	++
Total Chloride	+	++	--	-
Organic Chloride	++	++	+	++
Color Pt-Co	++	++	++	++
Density at 20°C	++	++	++	++
Distillation, IBP	+	+/-	++	++
Distillation, 50%	++	+	++	++
Distillation, DP	+	--	+	+
Total Nitrogen	-	-	+/-	-
Purity	+/-	--	+	++
Methylcyclohexane	n.e.	n.e.	-- *)	n.e.
Toluene	+	++	++	++
Nonaromatics	-	+	--	--
Solidification Point	+/-	--	+/-	-

table 8: comparison determinations on Benzene against the standards

	February 2015	February 2014	April 2013	April 2012
Acid Wash Color	++	+/-	n.e	n.e
Appearance	n.e.	n.e.	n.e	n.e
Color Pt-Co	+	++	++	++
Copper Corrosion	n.e.	n.e.	n.e	n.e
Density at 20 °C	++	++	++	++
Distillation, IBP	++	++	-	++
Distillation, 50%	+	+	-	++
Distillation, DP	-	--	++	++
Purity	+	-	+/-	++
Benzene	+ *)	+/- *)	- *)	-- *)
Nonaromatics	+	++	++	++

table 9: comparison determinations on Toluene against the standard
*) 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:

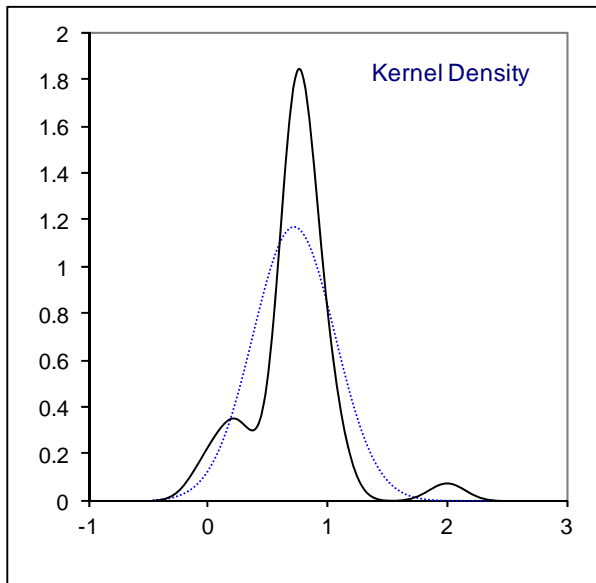
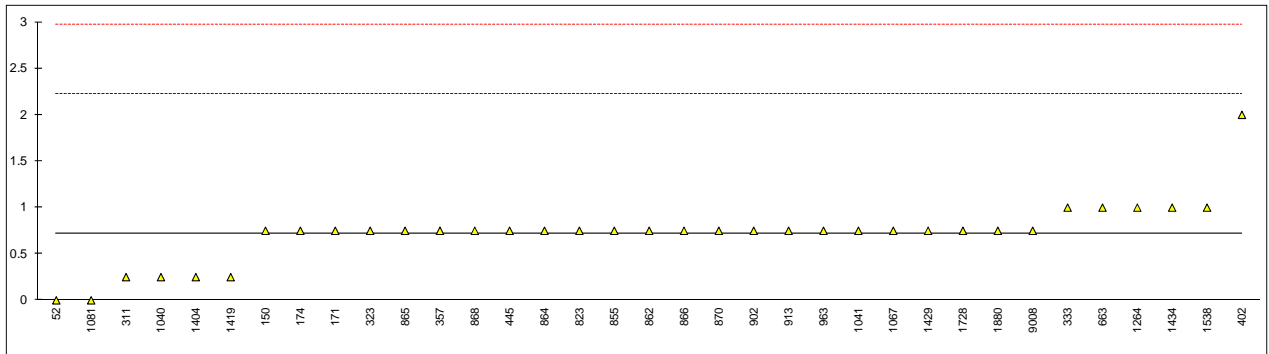
- ++: group performed much better than the standard
- + : group performed better than the standard
- +/-: group performance equals the standard
- : group performed worse than the standard
- : group performed much worse than the standard
- n.e.: not evaluated

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APPENDIX 1**Determination of Acid Wash Color on Benzene sample #15013**

lab	method	value	mark	z(targ)	remarks
52	D848	0		-0.96	
150	D848	1-		0.04	
171	D848	1-		0.04	
174	D848	1-		0.04	
311	D848	0+		-0.63	
322		----		----	
323	D848	-1		0.04	
333	D848	1		0.37	
334		----		----	
336		----		----	
337		----		----	
347		----		----	
357	D848	1-		0.04	
402	D848	2		1.71	
444		----		----	
445	D848	1-		0.04	
551		----		----	
555		----		----	
663	D848	1		0.37	
823	D848	1-		0.04	
855	D848	1-		0.04	
862	D848	1-		0.04	
864	D848	1-		0.04	
865	D848	1-		0.04	
866	D848	1-		0.04	
868	D848	1-		0.04	
870	D848	1-		0.04	
902	D848	1-		0.04	
912		----		----	
913	D848	<1		0.04	
963	D848	1-		0.04	
1040	D848	0+		-0.63	
1041	D848	1-		0.04	
1067	D848	1-		0.04	
1081	D848	0		-0.96	
1117		----		----	
1151		----		----	
1252		----		----	
1264	D848	1		0.37	
1294		----		----	
1404	D848	0+		-0.63	
1419	D848	0+		-0.63	
1429	D848	1-		0.04	
1434	D848	1		0.37	
1467		----		----	
1508		----		----	
1538	D848	1		0.37	
1653		----		----	
1657		----		----	
1728	D848	1-		0.04	
1812		----		----	
1823		----		----	
1846		----		----	
1866		----		----	
1880	D848	<1		0.04	
9008	D848	1-		0.04	
	normality	not OK			
	n	35			
	outliers	0			
	mean (n)	0.72 (1-)			
	st.dev. (n)	0.342			
	R(calc.)	0.96			
	R(D848:14)	2.10			

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



Determination of Acidity on Benzene sample #15013; results in mg NaOH per 100mL

lab	method	value	mark	z(targ)	remarks
52	D847	0		----	
150	D847	<0.001		----	
171	D847	NFA		----	
174	D847	NFA		----	
311	D847	NFA		----	
322				----	
323	D847	NFA		----	
333	D847	0		----	
334				----	
336				----	
337				----	
347	D847	NFA		----	
357	D847	NFA		----	
402	D847	NFA		----	
444				----	
445	D847	NFA		----	
551				----	
555				----	
663	D847	NFA		----	
823	D847	NFA		----	
855	D847	NFA		----	
862	D847	NFA		----	
864	D847	NFA		----	
865				----	
866	D847	NFA		----	
868	D847	NFA		----	
870	D847	NFA		----	
902	D847	NFA		----	
912				----	
913	D847	NFA		----	
963	D847	NFA		----	
1040				----	
1041				----	
1067	D847	NFA		----	
1081	D847	0		----	
1117	D847	0.3		----	
1151				----	
1252				----	
1264	D847	0		----	
1294				----	
1404				----	
1419				----	
1429	D847	NFA		----	
1434	D847	0		----	
1467				----	
1508				----	
1538	D847	NFA		----	
1653				----	
1657				----	
1728	D847	Absent		----	
1812				----	
1823	D847	NFA		----	
1846				----	
1866				----	
1880	D847	NFA		----	
9008				----	
	normality	n.a.			
	n	35			
	outliers	n.a.			
	mean (n)	No acid present			
	st.dev. (n)	n.a.			
	R(calc.)	n.a.			
	R(D847:08)	n.a.			

Abbreviation

NFA = No Free Acid

Determination of Appearance on Benzene sample #15013

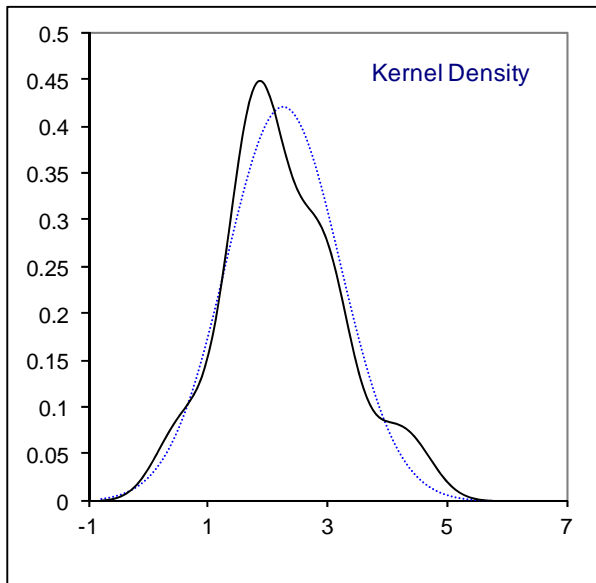
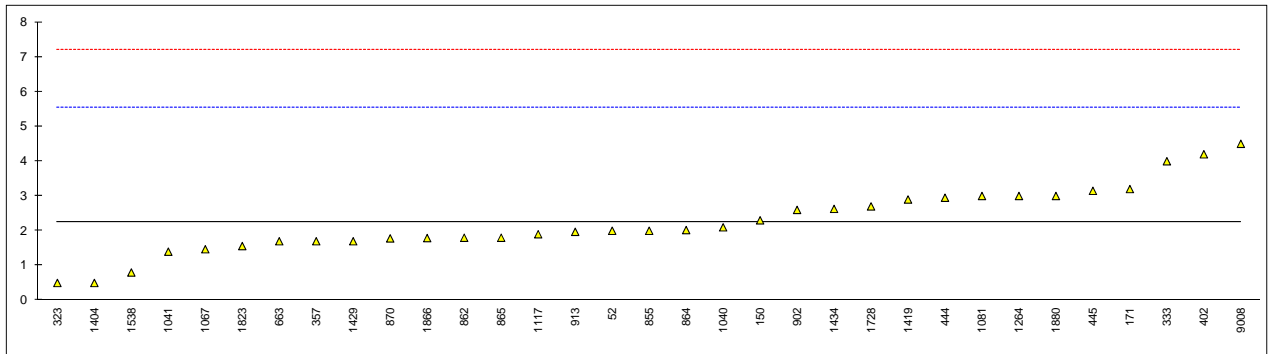
lab	method	value	mark	z(targ)	remarks
52	Visual	Pass		----	
150	E2680	C&B		----	
171	Visual	C&F		----	
174	E2680	Pass		----	
311	INH-402	C&B		----	
322		----		----	
323	Visual	C&B		----	
333	D4176	Pass		----	
334		----		----	
336	Visual	C&B		----	
337	Visual	Clear		----	
347	E2680	Pass		----	
357	E2680	Pass		----	
402	Visual	C&FFSM		----	
444	E2680	Pass		----	
445	E2680	Pass		----	
551		----		----	
555		----		----	
663	Visual	C&B		----	
823	E2680	Pass		----	
855	E2680	Pass		----	
862		----		----	
864	E2680	Pass		----	
865	E2680	Pass		----	
866	E2680	Pass		----	
868	E2680	Pass		----	
870	E2680	Pass		----	
902	E2680	Pass		----	
912		----		----	
913	Visual	Clear		----	
963	E2680	Pass		----	
1040	D4176	C&B		----	
1041		----		----	
1067	E2680	Pass		----	
1081	Visual	C&B		----	
1117	D4176	C&FFSM		----	
1151		----		----	
1252		----		----	
1264	Visual	Clear		----	
1294		----		----	
1404		----		----	
1419		----		----	
1429	E2680	C&B		----	
1434	Visual	Clear		----	
1467		Clear		----	
1508		----		----	
1538		C&B		----	
1653		----		----	
1657		----		----	
1728	Visual	Clear		----	
1812		----		----	
1823	Visual	C&FFSM		----	
1846		----		----	
1866		C&B		----	
1880		Clear		----	
9008		Clear		----	
	normality	n.a.			
	n	39			
	outliers	n.a.			
	mean (n)	Pass (C&B)			
	st.dev. (n)	n.a.			
	R(calc.)	n.a.			
	R(E2680:09e1)	n.a.			

Abbreviations:

C&B = clear and bright
C&F = clear and free
C&FFSM = clear and free from suspended matter

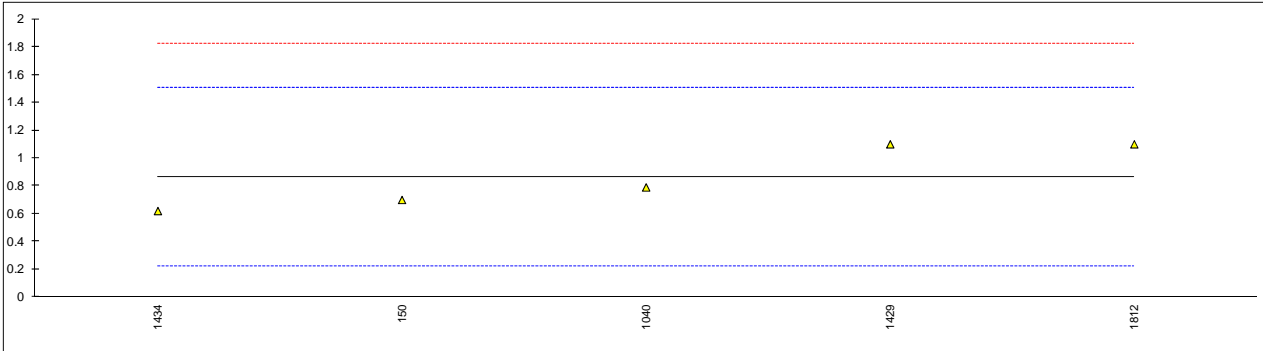
Determination of Bromine Index on Benzene sample #15013; results in mg Br/100g

	labmethod	value	mark	z(targ)remarks
52	D1492	2.0		-0.16
150	D1492	2.3		0.02
171	D5776	3.2		0.57
174		----		----
311	D5776	<0.5		----
322		----		----
323	D5776	0.5		-1.07
333	D5776	4.0		1.06
334		----		----
336		----		----
337		----		----
347		----		----
357	D5776	1.7		-0.34
402	D5776	4.2		1.18
444	D5776	2.95		0.42
445	D2710	3.15		0.54
551		----		----
555		----		----
663	D5776	1.7		-0.34
823		----		----
855	D5776	2.0		-0.16
862	D5776	1.8		-0.28
864	D5776	2.02		-0.15
865	D5776	1.8		-0.28
866	D5776	<10		----
868	D5776	<10		----
870	D5776	1.78		-0.29
902	D5776	2.6		0.21
912		----		----
913	D5776	1.97		-0.18
963		----		----
1040	DIN51774	2.1		-0.10
1041	D51774	1.4		-0.52
1067	D5776	1.47		-0.48
1081	D1492	3.0		0.45
1117	D1492	1.9		-0.22
1151		----		----
1252		----		----
1264	D1492	3.0		0.45
1294		----		----
1404	D5776	0.5		-1.07
1419	D1492	2.9		0.39
1429	D2710	1.7		-0.34
1434	D5776	2.63		0.22
1467		----		----
1508		----		----
1538	D1492	0.8		-0.89
1653		----		----
1657		----		----
1728	D1492	2.7		0.27
1812		----		----
1823	D1492	1.56		-0.43
1846		----		----
1866	D5776	1.79		-0.29
1880	D1492	3.0		0.45
9008	D5776	4.5		1.36
	normality	OK		
	n	33		
	outliers	0		
	mean (n)	2.26		
	st.dev. (n)	0.950		
	R(calc.)	2.66		
	R(D5776:14a)	4.60		



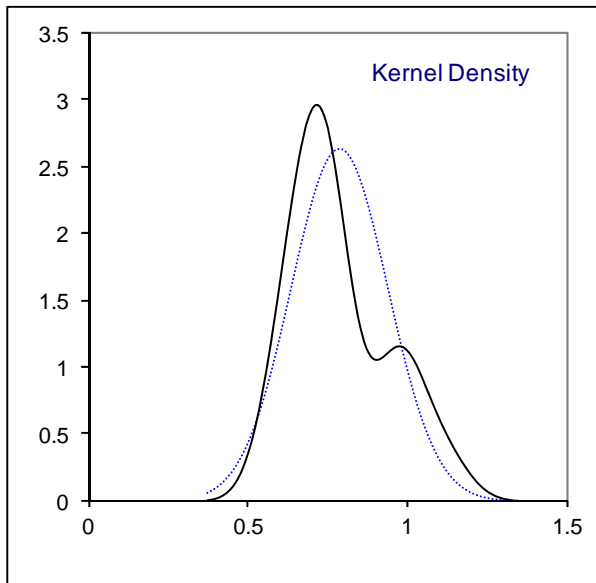
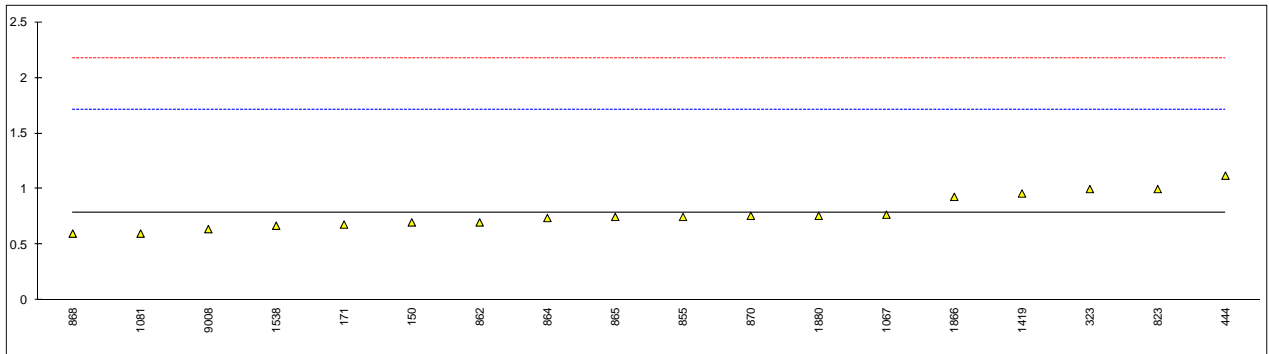
Determination of Total Chloride on Benzene sample #15013; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52		----		----	
150	D7359	0.7		-0.50	
171		----		----	
174		----		----	
311		----		----	
322		----		----	
323		----		----	
333		----		----	
334		----		----	
336		----		----	
337		----		----	
347		----		----	
357		----		----	
402		----		----	
444		----		----	
445		----		----	
551		----		----	
555		----		----	
663		----		----	
823		----		----	
855		----		----	
862		----		----	
864		----		----	
865		----		----	
866		----		----	
868		----		----	
870		----		----	
902		----		----	
912		----		----	
913		----		----	
963		----		----	
1040	EN14077	0.79		-0.22	
1041		----		----	
1067		----		----	
1081		----		----	
1117		----		----	
1151		----		----	
1252		----		----	
1264		----		----	
1294		----		----	
1404		----		----	
1419		----		----	
1429	D7359	1.1		0.74	
1434	D7536	0.62		-0.75	
1467		----		----	
1508		----		----	
1538		----		----	
1653		----		----	
1657		----		----	
1728		----		----	
1812	DIN51408	1.10		0.74	
1823		----		----	
1846		----		----	
1866		----		----	
1880		----		----	
9008		----		----	
	normality	unknown			
	n	5			
	outliers	0			
	mean (n)	0.862			
	st.dev. (n)	0.2254			
	R(calc.)	0.631			
	R(D5194:13)	0.900			



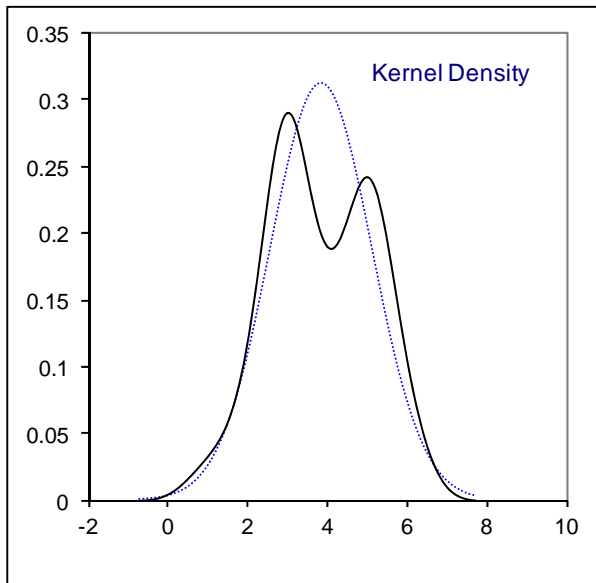
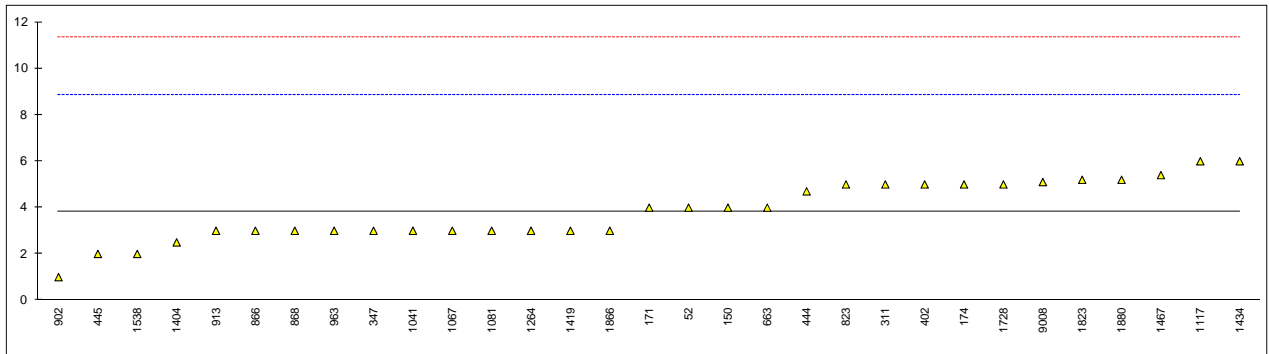
Determination of Organic Chlorides on Benzene sample #15013; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52		----		----	
150	D7359	0.7		-0.18	
171	D5808	0.681		-0.22	
174		----		----	
311	D5808	<1		----	
322		----		----	
323	D5808	1		0.46	
333		----		----	
334		----		----	
336		----		----	
337		----		----	
347	INH-1095	<1		----	
357		----		----	
402	D5808	<1		----	
444	IP510	1.12		0.72	
445	IP510	<2		----	
551		----		----	
555		----		----	
663	D5808	<1		----	
823	D5808	1		0.46	
855	D5808	0.75		-0.08	
862	D5808	0.7		-0.18	
864	D5808	0.74		-0.10	
865	D5808	0.75		-0.08	
866		----		----	
868	D5808	0.6		-0.40	
870	D5808	0.76		-0.05	
902		----		----	
912		----		----	
913		----		----	
963		----		----	
1040		----		----	
1041		----		----	
1067	UOP779	0.77		-0.03	
1081	D5808	0.6		-0.40	
1117		----		----	
1151		----		----	
1252		----		----	
1264		----		----	
1294		----		----	
1404		----		----	
1419	EN14077	0.96		0.38	
1429		----		----	
1434		----		----	
1467		----		----	
1508		----		----	
1538	D5808	0.67		-0.25	
1653		----		----	
1657		----		----	
1728		----		----	
1812		----		----	
1823		----		----	
1846		----		----	
1866	D5808	0.93		0.31	
1880	D5808	0.76		-0.05	
9008	D5808	0.64		-0.31	
	normality	OK			
	n	18			
	outliers	0			
	mean (n)	0.785			
	st.dev. (n)	0.1515			
	R(calc.)	0.424			
	R(D5808:09a)	1.300			
				<u>Spike</u>	
				0.78	Recovery <100%



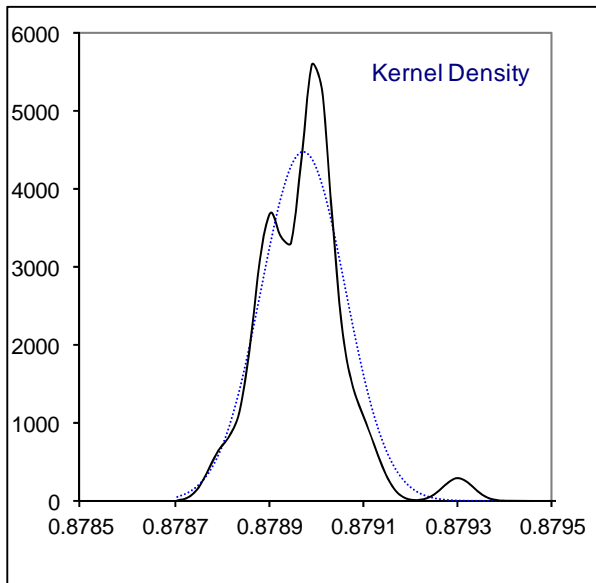
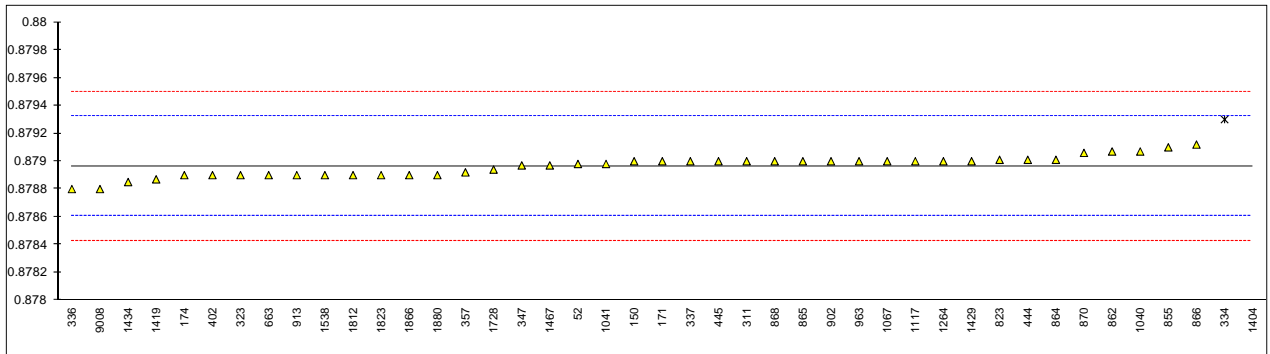
Determination of Colour (Pt-Co scale) on Benzene sample #15013

lab	method	value	mark	z(targ)	remarks
52	D5386	4		0.06	
150	D1209	4		0.06	
171	D1209	4		0.06	
174	D1209	5		0.46	
311	D1209	5		0.46	
322		----		----	
323	D1209	<5		----	
333		----		----	
334		----		----	
336		----		----	
337		----		----	
347	D5386	3		-0.34	
357	D1209	<5		----	
402	D1209	5		0.46	
444	D5386	4.7		0.34	
445	D1209	2		-0.74	
551		----		----	
555		----		----	
663	D1209	4		0.06	
823	D5386	5		0.46	
855	D1209	<5		----	
862	D1209	<5		----	
864	D1209	<5		----	
865	D1209	<5		----	
866	D1209	3		-0.34	
868	D1209	3		-0.34	
870	D1209	<5		----	
902	D5386	1		-1.14	
912		----		----	
913	D5386	3		-0.34	
963	D1209	3		-0.34	
1040	ISO6271	<5		----	
1041	ISO6271	3	C	-0.34	First reported: 11
1067	D5386	3		-0.34	
1081	D5386	3.0		-0.34	
1117	D1209	6		0.86	
1151		----		----	
1252		----		----	
1264	D1209	3.0		-0.34	
1294		----		----	
1404	D1209	2.5		-0.54	
1419	D1209	3		-0.34	
1429	D1209	<5		----	
1434	D1209	6		0.86	
1467	in house	5.4		0.62	
1508		----		----	
1538	D1209	2		-0.74	
1653		----		----	
1657		----		----	
1728	D1209	5		0.46	
1812		----		----	
1823	D1209	5.2		0.54	
1846		----		----	
1866	D1209	3		-0.34	
1880	D5386	5.2		0.54	
9008	D1209	5.1		0.50	
	normality	OK			
	n	31			
	outliers	0			
	mean (n)	3.84			
	st.dev. (n)	1.278			
	R(calc.)	3.58			
	R(D1209:05e1)	7.00			Compare R(D5386:10) = 5.2



Determination of Density at 20°C on Benzene sample #15013; results in kg/L

lab	method	value	mark	z(targ)	remarks
52	D4052	0.87898		0.09	
150	D4052	0.8790		0.20	
171	D4052	0.8790		0.20	
174	D4052	0.8789		-0.36	
311	D4052	0.8790		0.20	
322		----		----	
323	D4052	0.8789		-0.36	
333		----		----	
334	ISO12185	0.8793	R(0.01)	1.88	
336	ISO12185	0.8788		-0.92	
337	ISO12185	0.8790		0.20	
347	D4052	0.87897		0.03	
357	ISO12185	0.87892		-0.25	
402	ISO12185	0.8789		-0.36	
444	D4052	0.87901		0.26	
445	D4052	0.8790		0.20	
551		----		----	
555		----		----	
663	D4052	0.8789		-0.36	
823	ISO12185	0.87901		0.26	
855	D4052	0.87910		0.76	
862	D4052	0.87907		0.59	
864	D4052	0.87901		0.26	
865	D4052	0.8790		0.20	
866	D4052	0.87912		0.87	
868	D4052	0.87900		0.20	
870	D4052	0.87906		0.54	
902	D4052	0.8790		0.20	
912		----		----	
913	D4052	0.8789		-0.36	
963	ISO12185	0.8790		0.20	
1040	ISO12185	0.87907		0.59	
1041	ISO12185	0.87898	C	0.09	first reported: 878.98
1067	ISO12185	0.8790		0.20	
1081		----		----	
1117	D4052	0.8790		0.20	
1151		----		----	
1252		----		----	
1264	D4052	0.8790		0.20	
1294		----		----	
1404	ISO12185	0.8842	ex	29.32	measured at 15°C, excluded, see §4.1
1419	ISO12185	0.87887	C	-0.53	first reported: 878.87
1429	D4052	0.8790		0.20	
1434	D4052	0.87885		-0.64	
1467	D4052	0.87897	C	0.03	first reported: 878.97
1508		----		----	
1538	ISO12185	0.8789		-0.36	
1653		----		----	
1657		----		----	
1728	ISO12185	0.87894		-0.13	
1812	ISO12185	0.8789	C	-0.36	first reported: 0.8669
1823	D4052	0.8789	C	-0.36	first reported: 878.9
1846		----		----	
1866	ISO12185	0.8789		-0.36	
1880	D4052	0.8789		-0.36	
9008	D4052	0.8788		-0.92	
	normality	OK			
	n	41			
	outliers	1 (+1ex)			
	mean (n)	0.87896			
	st.dev. (n)	0.000074			
	R(calc.)	0.00020			
	R(D4052:02e1)	0.00050			



Determination of Distillation on Benzene sample #15013; results in °C

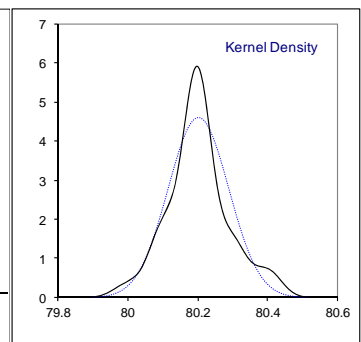
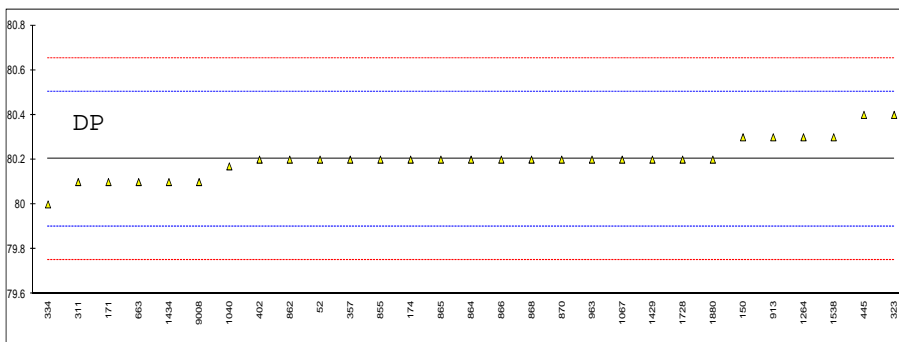
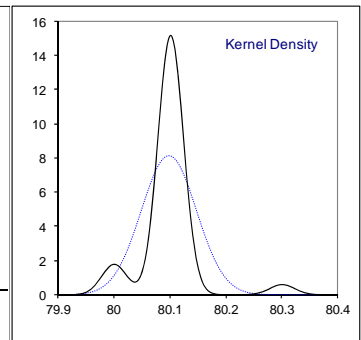
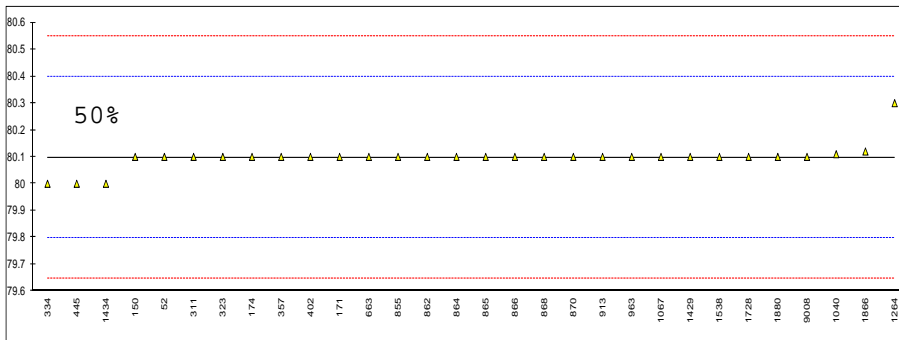
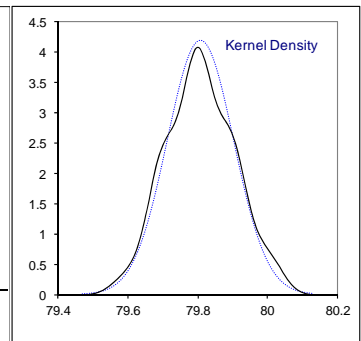
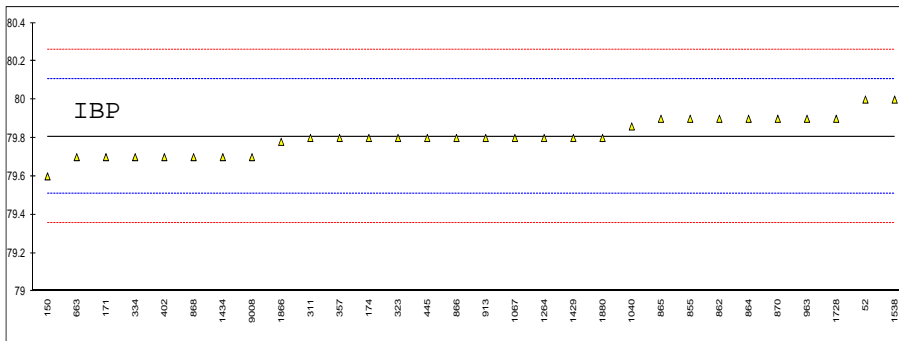
Lab	method	mode	IBP	mark	z(targ)	50%	mark	z(targ)	DP	mark	z(targ)
52	D850	Automated	80.0		1.28	80.1		0.02	80.2		-0.02
150	D850	Automated	79.6		-1.39	80.1		0.02	80.3		0.65
171	D850	Automated	79.7	C	-0.72	80.1		0.02	80.1		-0.68
174	D850	Automated	79.8		-0.05	80.1		0.02	80.2		-0.02
311	D850	Automated	79.8		-0.05	80.1		0.02	80.1		-0.68
322		----	----		----	----		----	----		----
323	D850	Manual	79.8		-0.05	80.1		0.02	80.4		1.32
333		----	----		----	----		----	----		----
334	D850	Automated	79.7		-0.72	80.0		-0.65	80.0		-1.35
336		----	----		----	----		----	----		----
337		----	----		----	----		----	----		----
347		----	----		----	----		----	----		----
357	D850	Automated	79.8		-0.05	80.1		0.02	80.2		-0.02
402	D850	Manual	79.7		-0.72	80.1		0.02	80.2		-0.02
444		----	----		----	----		----	----		----
445	D850	Manual	79.8		-0.05	80.0		-0.65	80.4		1.32
551		----	----		----	----		----	----		----
555		----	----		----	----		----	----		----
663	D850	Automated	79.7		-0.72	80.1		0.02	80.1		-0.68
823		----	----		----	----		----	----		----
855	D850	Manual	79.9		0.61	80.1		0.02	80.2		-0.02
862	D850	Manual	79.9		0.61	80.1		0.02	80.2		-0.02
864	D850	Manual	79.9		0.61	80.1		0.02	80.2		-0.02
865	D850	Manual	79.9		0.61	80.1		0.02	80.2		-0.02
866	D850	Manual	79.8		-0.05	80.1		0.02	80.2		-0.02
868	D850	Manual	79.7		-0.72	80.1		0.02	80.2		-0.02
870	D850	Manual	79.9		0.61	80.1		0.02	80.2		-0.02
902		----	----		----	----		----	----		----
912		----	----		----	----		----	----		----
913	D850	Manual	79.8		-0.05	80.1		0.02	80.3		0.65
963	D850	Automated	79.9		0.61	80.1		0.02	80.2		-0.02
1040	DIN51761	Manual	79.86		0.35	80.11		0.08	80.17		-0.22
1041		----	----		----	----		----	----		----
1067	D850	Manual	79.8		-0.05	80.1		0.02	80.2		-0.02
1081		----	----		----	----		----	----		----
1117		----	----		----	----		----	----		----
1151		----	----		----	----		----	----		----
1252		----	----		----	----		----	----		----
1264	D850	Automated	79.8		-0.05	80.3		1.35	80.3		0.65
1294		----	----		----	----		----	----		----
1404		----	----		----	----		----	----		----
1419		----	----		----	----		----	----		----
1429	D850	Automated	79.8		-0.05	80.1		0.02	80.2		-0.02
1434	D850	Automated	79.7		-0.72	80.0		-0.65	80.1		-0.68
1467		----	----		----	----		----	----		----
1508		----	----		----	----		----	----		----
1538	D850	Automated	80.0		1.28	80.1		0.02	80.3		0.65
1653		----	----		----	----		----	----		----
1657		----	----		----	----		----	----		----
1728	D850	Manual	79.9		0.61	80.1		0.02	80.2		-0.02
1812		----	----		----	----		----	----		----
1823		----	----		----	----		----	----		----
1846		----	----		----	----		----	----		----
1866	D850	Automated	79.78		-0.19	80.12		0.15	----		----
1880	D850	Automated	79.8		-0.05	80.1		0.02	80.2		-0.02
9008	D850	Automated	79.7		-0.72	80.1		0.02	80.1		-0.68
	normality	Autom./Man.	OK			not OK			suspect		
	n	16/14	30			30			29		
	outliers		0			0			0		
	mean (n)		79.81			80.10			80.20		
	st.dev. (n)		0.095			0.049			0.087		
	R(calc.)		0.27			0.14			0.24		
	R(D850:11)		0.42			0.42			0.42		

Laboratory 171 first reported for Initial Boiling Point: 79.2

Theoretical mid boiling point = 80.1°C

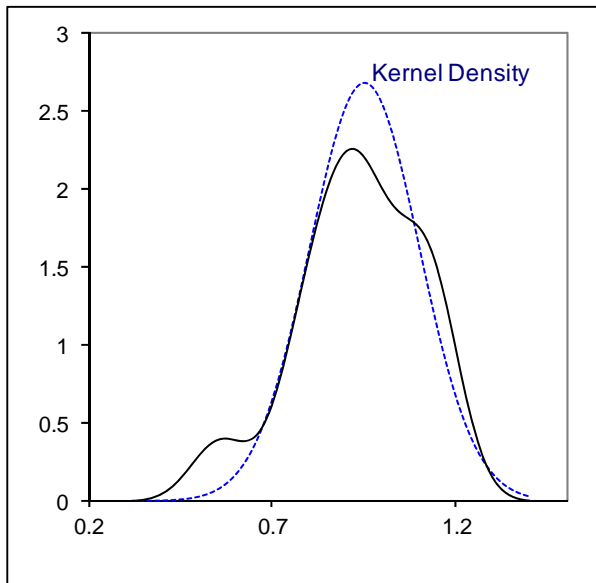
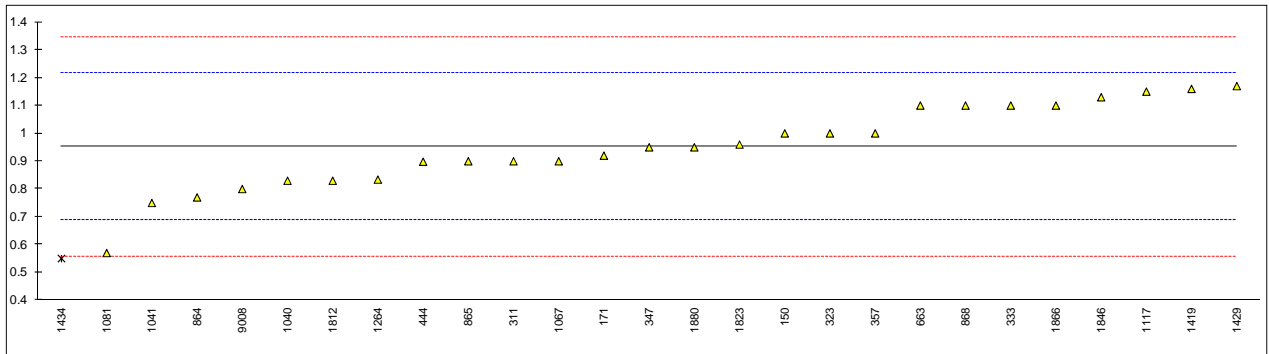
After manual correction:

1264 D850	Automated	79.6	-1.34	80.1	0.06	80.1	-0.64
normality		OK		not OK		suspect	
n		30		30		29	
outliers		0		0		0	
mean (n)		79.80		80.09		80.20	
st.dev. (n)		0.102		0.031		0.087	
R(calc.)		0.29		0.09		0.24	
R(D850:11)		0.42		0.42		0.42	



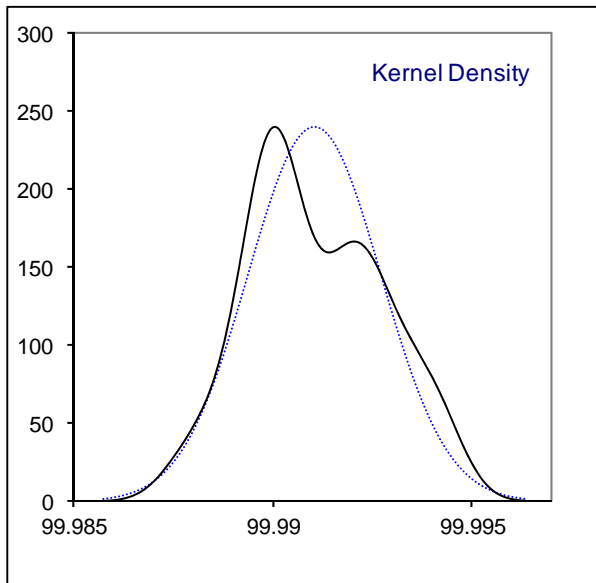
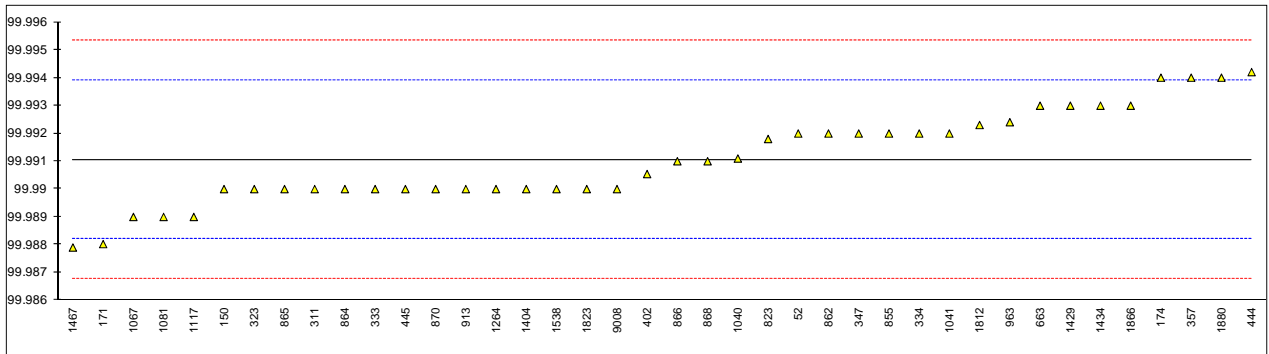
Determination of Total Nitrogen on Benzene sample #15013; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52		----		----	
150	D6069	1.0		0.36	
171	D4629	0.92		-0.25	
174		----		----	
311	D6069	0.9		-0.40	
322		----		----	
323	D6069	1.0		0.36	
333	D4629	1.1		1.12	
334		----		----	
336		----		----	
337		----		----	
347	D4629	0.95		-0.02	
357	D6069	1.0		0.36	
402		----		----	
444	D4629	0.898		-0.42	
445	D4629	<1		----	
551		----		----	
555		----		----	
663	D6069	1.1		1.12	
823		----		----	
855		----		----	
862		----		----	
864	D6069	0.77		-1.39	
865	D6069	0.90		-0.40	
866		----		----	
868	D6069	1.1		1.12	
870		----		----	
902		----		----	
912		----		----	
913		----		----	
963		----		----	
1040	D6069	0.83		-0.93	
1041	D6069	0.75		-1.54	
1067	D6069	0.90		-0.40	
1081	D6069	0.57		-2.91	
1117	D6069	1.15		1.50	
1151		----		----	
1252		----		----	
1264	D6069	0.834		-0.90	
1294		----		----	
1404	D6069	<1		----	
1419	D6069	1.16		1.58	
1429	D4629	1.17		1.65	
1434	D7184	0.55	ex	-3.06	
1467		----		----	
1508		----		----	
1538		----		----	
1653		----		----	
1657		----		----	
1728		----		----	
1812	D6069	0.83		-0.93	
1823	D6069	0.96		0.05	
1846	D4629	1.13		1.35	
1866	D6069	1.10		1.12	
1880	D6069	0.95		-0.02	
9008	D6069	0.8		-1.16	
	normality	OK			
	n	26			
	outliers	0 (+1ex)		<u>Spike</u>	
	mean (n)	0.953		0.81	Recovery <118%
	st.dev. (n)	0.1490			
	R(calc.)	0.417			
	R(D6069:01)	0.368			Application range D6069:01 = 0.2 – 2 mg/kg
Comp.	R(D4629:12)	0.789			Application range D4629:12 = 0.3 – 100 mg/kg



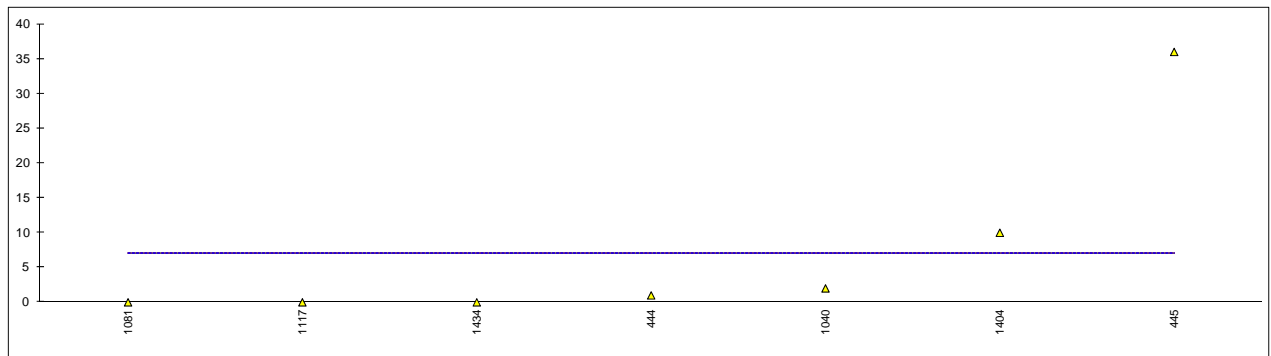
Determination of Purity on Benzene sample #15013; results in %M/M

lab	method	value	mark	z(targ)	remarks
52	D4492	99.992		0.66	
150	D4492	99.99		-0.74	
171	D4492	99.98802		-2.12	
174	D4492	99.994		2.06	
311	D4492	99.99		-0.74	
322		----		----	
323	D4492	99.99		-0.74	
333	D4492	99.99		-0.74	
334	D4492	99.992		0.66	
336		----		----	
337		----		----	
347	D4492	99.992		0.66	
357	D4492	99.994		2.06	
402	D4492	99.99054		-0.36	
444	D4492	99.9942		2.20	
445	D4492	99.99		-0.74	
551		----		----	
555		----		----	
663	D4492	99.993		1.36	
823	D4492	99.9918		0.52	
855	D4492	99.992		0.66	
862	D4492	99.992		0.66	
864	D4492	99.990		-0.74	
865	D4492	99.99		-0.74	
866	D4492	99.991		-0.04	
868	D4492	99.991		-0.04	
870	D4492	99.990		-0.74	
902		----		----	
912		----		----	
913	D4492	99.99		-0.74	
963	D4492	99.9924		0.94	
1040	D4492	99.9911		0.03	
1041	D4492	99.992		0.66	
1067	in house	99.989		-1.44	
1081	D4492	99.989		-1.44	
1117	D4492	99.989		-1.44	
1151		----		----	
1252		----		----	
1264	D4492	99.99		-0.74	
1294		----		----	
1404	D4492	99.99		-0.74	
1419		----		----	
1429	D4492	99.993		1.36	
1434	D4492	99.993		1.36	
1467	in house	99.9879		-2.21	
1508		----		----	
1538	D4492	99.99		-0.74	
1653		----		----	
1657		----		----	
1728		----		----	
1812	DIN51437	99.9923		0.87	
1823	D4492	99.99		-0.74	
1846		----		----	
1866	D4492	99.993		1.36	
1880	D4492	99.994		2.06	
9008	D4492	99.99		-0.74	
	normality	OK			
	n	40			
	outliers	0			
	mean (n)	99.9911			
	st.dev. (n)	0.00166			
	R(calc.)	0.0047			
	R(D4492:10)	0.0040			



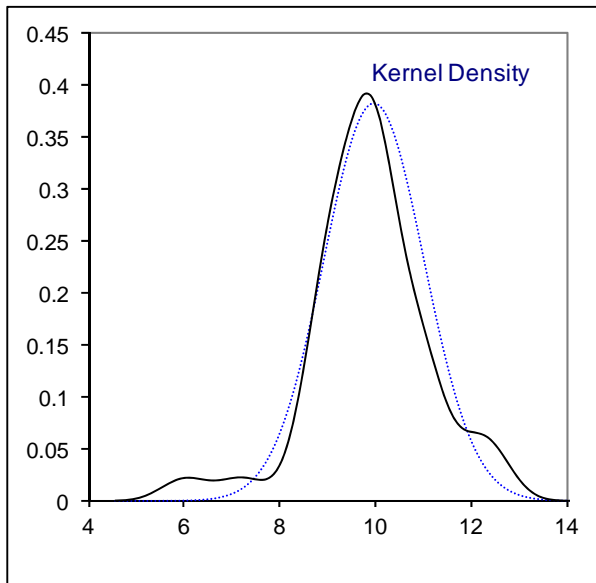
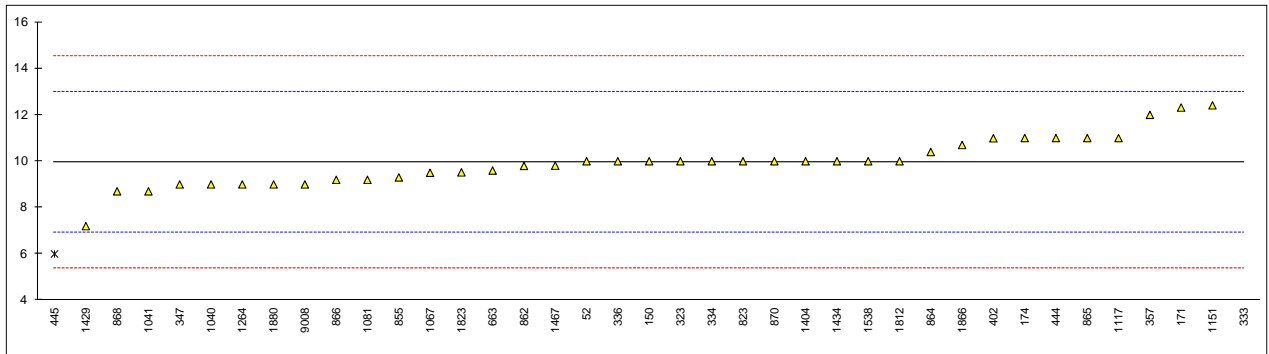
Determination of Methylcyclohexane on Benzene sample #15013 in mg/kg

lab	method	value	mark	z(targ)	remarks
52		----		----	
150	D4492	<10		----	
171	D4492	<10		----	
174	D4492	<10		----	
311	D5713	<2		----	
322		----		----	
323	D5713	<2		----	
333		----		----	
334		----		----	
336		----		----	
337		----		----	
347	D4492	<50		----	
357	D4492	<10		----	
402		----		----	
444	D5713	1		----	
445	D4492	36		----	false positive?
551		----		----	
555		----		----	
663		----		----	
823	D5713	<2		----	
855	D4492	<10		----	
862		----		----	
864	D4492	<10		----	
865	D4492	<10		----	
866	D5713	<10		----	
868	D4492	<10		----	
870	D4492	<10		----	
902		----		----	
912		----		----	
913	D4492	<10		----	
963	D4492	<50		----	
1040	D4492	2		----	
1041	in house	<5		----	
1067	in house	<5		----	
1081	D5713	0		----	
1117	D4492	0		----	
1151		----		----	
1252		----		----	
1264	D4492	<1		----	
1294		----		----	
1404		10		----	
1419		----		----	
1429	D4492	<10		----	
1434	D4492	0		----	
1467		----		----	
1508		----		----	
1538		----		----	
1653		----		----	
1657		----		----	
1728		----		----	
1812	DIN51437	<5		----	
1823		----		----	
1846		----		----	
1866		----		----	
1880		----		----	
9008		----		----	
	normality	unknown			
	n	24			
	outliers	n.a.			
	mean (n)	<10			
	st.dev. (n)	n.a.			
	R(calc.)	n.a.			
	R(lit)	n.a.			



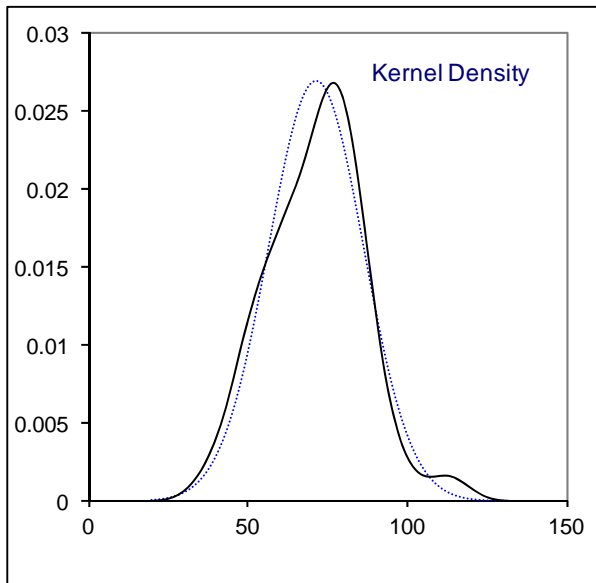
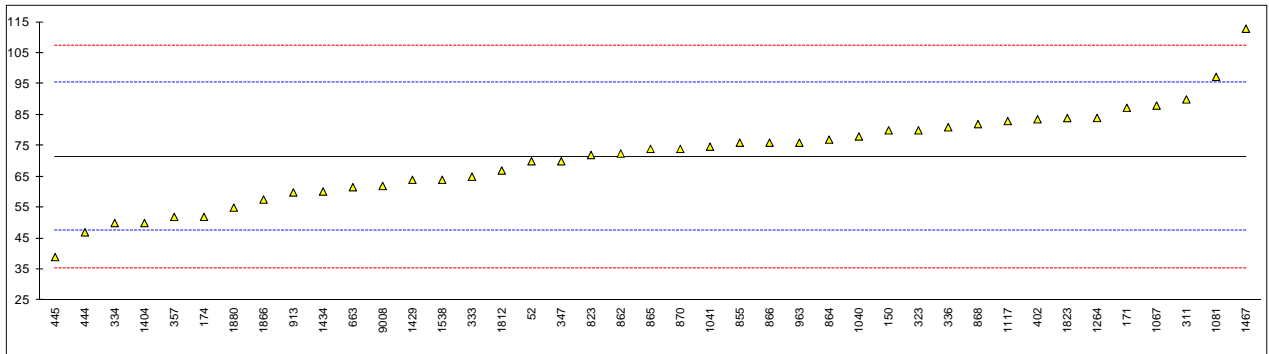
Determination of Toluene on Benzene sample #15013; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D4492	10		0.03	
150	D4492	10		0.03	
171	D4492	12.315		1.55	
174	D4492	11		0.69	
311	D4492	<10		----	
322		----		----	
323	D4492	10		0.03	
333	D4492	40	R(0.01)	19.72	
334	D4492	10	C	0.03	first reported: 0.001
336	UOP744	10		0.03	
337		----		----	
347	D4492	9		-0.63	
357	D4492	12		1.34	
402	D4492	10.99		0.68	
444	D5713	11		0.69	
445	D4492	6	R(0.05)	-2.60	
551		----		----	
555		----		----	
663	D4492	9.6		-0.23	
823	D4492	10		0.03	
855	D4492	9.3		-0.43	
862	D4492	9.8		-0.10	
864	D4492	10.4		0.29	
865	D4492	11		0.69	
866	D4492	9.2		-0.50	
868	D4492	8.7		-0.82	
870	D4492	10		0.03	
902		----		----	
912		----		----	
913	D4492	<10		----	
963	D4492	<10		----	
1040	D4492	9		-0.63	
1041	D4492	8.7		-0.82	
1067	in house	9.5		-0.30	
1081	D4492	9.2		-0.50	
1117	D4492	11		0.69	
1151	in house	12.41		1.61	
1252		----		----	
1264	D4492	9		-0.63	
1294		----		----	
1404	D4492	10		0.03	
1419		----		----	
1429	D4492	7.2		-1.81	
1434	D4492	10		0.03	
1467	in house	9.81		-0.10	
1508		----		----	
1538	D4492	10		0.03	
1653		----		----	
1657		----		----	
1728		----		----	
1812	DIN51437	10		0.03	
1823	D4492	9.52		-0.29	
1846		----		----	
1866	D4492	10.7		0.49	
1880	D4492	9		-0.63	
9008	D4492	9		-0.63	
	normality	suspect			
	n	37			
	outliers	2			
	mean (n)	9.96			
	st.dev. (n)	1.047			
	R(calc.)	2.93			
	R(D4492:10)	4.27			



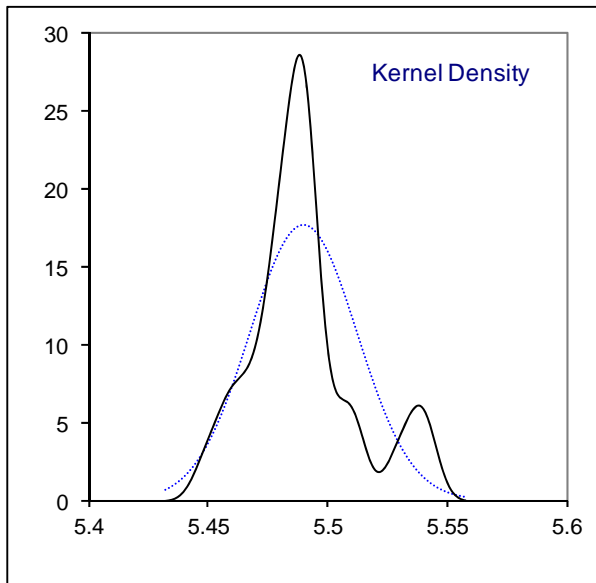
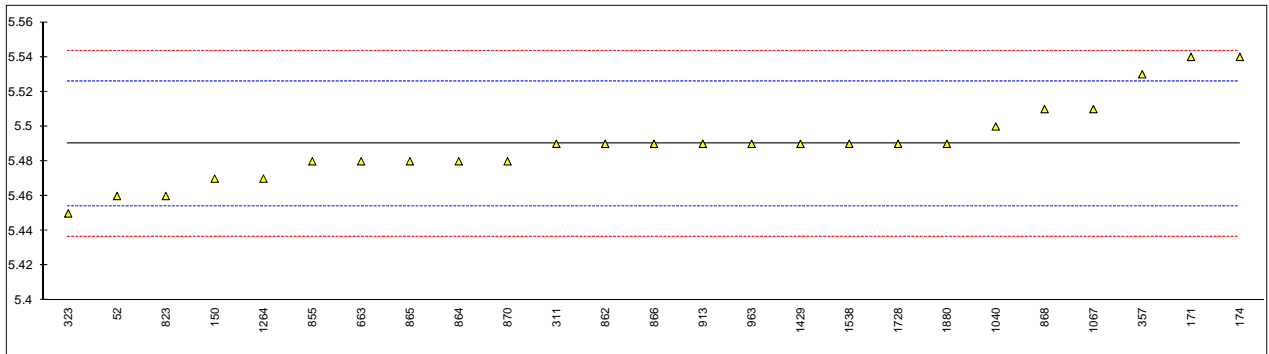
Determination of Nonaromatics on Benzene sample #15013; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D4492	70		-0.12	
150	D4492	80		0.71	
171	D4492	87.3		1.32	
174	D4492	52		-1.62	
311	D4492	90		1.54	
322		----		----	
323	D4492	80		0.71	
333	D4492	65		-0.54	
334	D4492	50	C	-1.79	first reported: 0.005
336	UOP744	81		0.80	
337		----		----	
347	D4492	70		-0.12	
357	D4492	52		-1.62	
402	D4492	83.58		1.01	
444	D4492	47	C	-2.04	first reported: 1
445	D4492	39		-2.70	
551		----		----	
555		----		----	
663	D4492	61.6		-0.82	
823	D4492	72		0.05	
855	D4492	76.0		0.38	
862	D4492	72.5		0.09	
864	D4492	77		0.46	
865	D4492	74		0.21	
866	D4492	76		0.38	
868	D4492	82		0.88	
870	D4492	74		0.21	
902		----		----	
912		----		----	
913	D4492	59.9		-0.96	
963	D4492	76		0.38	
1040	D4492	78		0.55	
1041	D4492	74.7		0.27	
1067	in house	88		1.38	
1081	D4492	97.3		2.15	
1117	D4492	83		0.96	
1151		----		----	
1252		----		----	
1264	D4492	84		1.05	
1294		----		----	
1404	D4492	50		-1.79	
1419		----		----	
1429	D4492	64		-0.62	
1434	D4492	60.2		-0.94	
1467	in house	112.85		3.45	
1508		----		----	
1538	D4492	64		-0.62	
1653		----		----	
1657		----		----	
1728		----		----	
1812	DIN51437	67		-0.37	
1823	D4492	83.96		1.04	
1846		----		----	
1866	D4492	57.6		-1.15	
1880	D4492	55		-1.37	
9008	D4492	62		-0.79	
	normality	OK			
	n	41			
	outliers	0			
	mean (n)	71.45			
	st.dev. (n)	14.806			
	R(calc.)	41.46			
	R(D4492:10)	33.62			



Determination of Solidification Point (anhydrous) on Benzene sample #15013; results in °C

lab	method	value	mark	z(targ)	remarks
52	D852	5.46		-1.68	
150	D852	5.47		-1.12	
171	D852	5.54		2.80	
174	D852	5.54		2.80	
311	D852	5.49		0.00	
322		----		----	
323	D852	5.45		-2.24	
333		----		----	
334		----		----	
336		----		----	
337		----		----	
347		----		----	
357	D852	5.53		2.24	
402		----		----	
444		----		----	
445		----		----	
551		----		----	
555		----		----	
663	D852	5.48		-0.56	
823	D852	5.46		-1.68	
855	D852	5.48		-0.56	
862	D852	5.49		0.00	
864	D852	5.48		-0.56	
865	D852	5.48		-0.56	
866	D852	5.49		0.00	
868	D852	5.51		1.12	
870	D852	5.48		-0.56	
902		----		----	
912		----		----	
913	D852	5.49		0.00	
963	D852	5.49		0.00	
1040	DIN51798	5.50		0.56	
1041		----		----	
1067	D852	5.51		1.12	
1081		----		----	
1117		----		----	
1151		----		----	
1252		----		----	
1264	D852	5.47		-1.12	
1294		----		----	
1404		----		----	
1419		----		----	
1429	D852	5.49		0.00	
1434		----		----	
1467		----		----	
1508		----		----	
1538	D852	5.49		0.00	
1653		----		----	
1657		----		----	
1728	D852	5.49		0.00	
1812		----		----	
1823		----		----	
1846		----		----	
1866		----		----	
1880	D852	5.49		0.00	
9008		----		----	
	normality	OK			
	n	25			
	outliers	0			
	mean (n)	5.490			
	st.dev. (n)	0.0225			
	R(calc.)	0.063			
	R(D852:13)	0.050			

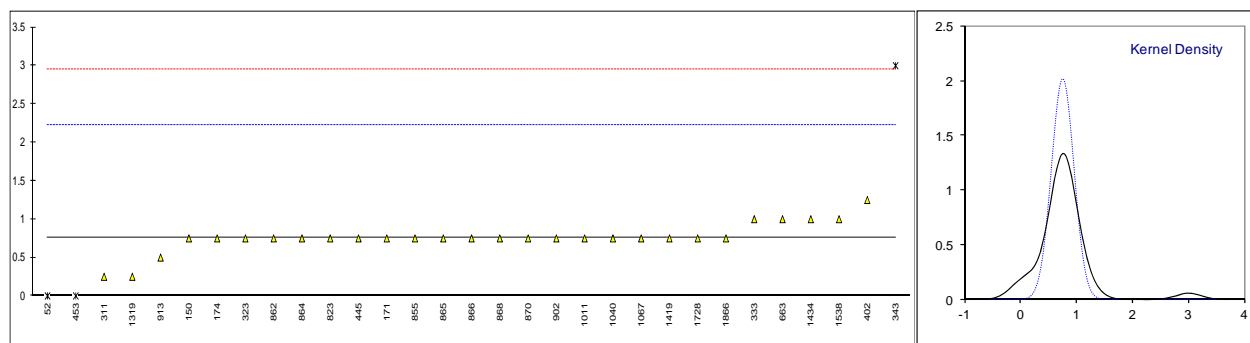


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Determination of Acid Wash Color on Toluene sample #15014

lab	method	value	mark	z(targ)	remarks
52	D848	0	R(0.05)	-1.04	
150	D848	1-		-0.01	
171	D848	1-		-0.01	
174	D848	1-		-0.01	
311	D848	0+		-0.70	
323	D848	1-		-0.01	
333	D848	1		0.33	
334		----		----	
343	D848	3	R(0.01)	3.06	
402	D848	1+		0.67	
445	D848	1-		-0.01	
453	D848	0	R(0.05)	-1.04	
551		----		----	
555		----		----	
663	D848	1		0.33	
823	D848	1-		-0.01	
855	D848	1-		-0.01	
862	D848	1-		-0.01	
864	D848	1-		-0.01	
865	D848	1-		-0.01	
866	D848	1-		-0.01	
868	D848	1-		-0.01	
870	D848	1-		-0.01	
902	D848	1-		-0.01	
912		----		----	
913	D848	<1.0		-0.35	
1011	D848	1-		-0.01	
1040	D848	1-		-0.01	
1041		----		----	
1067	D848	1-		-0.01	
1151		----		----	
1319	D848	0+		-0.70	
1419	D848	1-		-0.01	
1434	D848	1		0.33	
1538	D848	1		0.33	
1728	D848	1-		-0.01	
1812		----		----	
1843		----		----	
1866	D848	1-		-0.01	
7002		----		----	
normality		not OK			
n		28			
outliers		3			
mean (n)		0.76 (1-)			
st.dev. (n)		0.198			
R(calc.)		0.55			
R(D848:14)		2.05			

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



Determination of Appearance on Toluene sample #15014

lab	method	value	mark	z(targ)	remarks
52	Visual	Pass		----	
150	E2680	C&B		----	
171	E2680	C&F		----	
174	E2680	Pass		----	
311	INH-402	C&B		----	
323	Visual	C&B		----	
333		----		----	
334		----		----	
343	E2680	Pass		----	
402	Visual	CFSM		----	
445	E2680	Pass		----	
453	D4176	C&B		----	
551		----		----	
555		----		----	
663	Visual	C&B		----	
823	E2680	Pass		----	
855	E2680	Pass		----	
862		----		----	
864	E2680	Pass		----	
865	E2680	Pass		----	
866	E2680	Pass		----	
868	E2680	Pass		----	
870	E2680	Pass		----	
902	E2680	Pass		----	
912		----		----	
913	Visual	Clear		----	
1011	Visual	C&B		----	
1040	D4176	C&B		----	
1041		----		----	
1067	E2680	Pass		----	
1151		----		----	
1319	D841	CFSH		----	
1419		----		----	
1434	Visual	Clear		----	
1538		C&B		----	
1728	Visual	Clear		----	
1812		----		----	
1843	in house	CFSH		----	
1866		C&B		----	
7002		Pass		----	
	normality	n.a.			
	n	30			
	outliers	n.a.			
	mean (n)	Pass (C&B)			
	st.dev. (n)	n.a.			
	R(calc.)	n.a.			
	R(E2680:09e1)	Unknown			

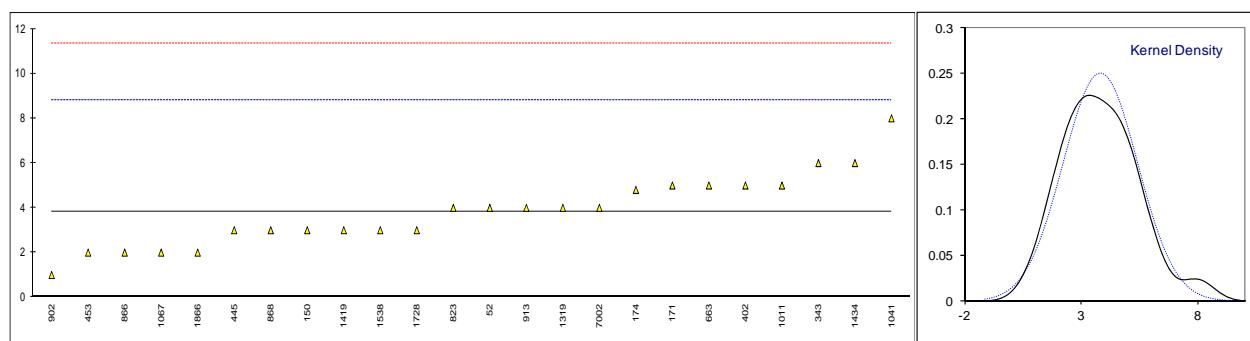
Abbreviations:

C&B	= clear and bright
C&F	= clear and free
CFSM	= clear and free from suspended matter
CFSH	= clear liquid free from sediment and haze

Determination of Colour (Pt-Co scale) on Toluene sample #15014

lab	method	value	mark	z(targ)	remarks
52	D5386	4		0.07	
150	D1209	3		-0.33	
171	D1209	5		0.47	
174	D1209	4.8		0.39	
311	D1209	<5		----	
323	D1209	<5		----	
333		----		----	
334		----		----	
343	D5386	6		0.87	
402	D1209	5.0		0.47	
445	D1209	3		-0.33	
453	D5386	2		-0.73	
551		----		----	
555		----		----	
663	D1209	5		0.47	
823	D5386	4		0.07	
855	D1209	<5		----	
862	D1209	<5		----	
864	D1209	<5		----	
865	D1209	<5		----	
866	D1209	2		-0.73	
868	D1209	3		-0.33	
870	D1209	<5		----	
902	D5386	1		-1.13	
912		----		----	
913	D5386	4		0.07	
1011	D1209	5		0.47	
1040	ISO6271	<5		----	
1041	ISO6271	8		1.67	
1067	D5386	2		-0.73	
1151		----		----	
1319	D1209	4		0.07	
1419	D1209	3		-0.33	
1434	D1209	6		0.87	
1538	D1209	3		-0.33	
1728	D1209	3		-0.33	
1812		----		----	
1843		----		----	
1866	D1209	2		-0.73	
7002	D1209	4		0.07	
normality		OK			
n		24			
outliers		0			
mean (n)		3.83			
st.dev. (n)		1.600			
R(calc.)		4.48			
R(D1209:05e1)		7.00			

Compare R(D5386:10) = 5.19

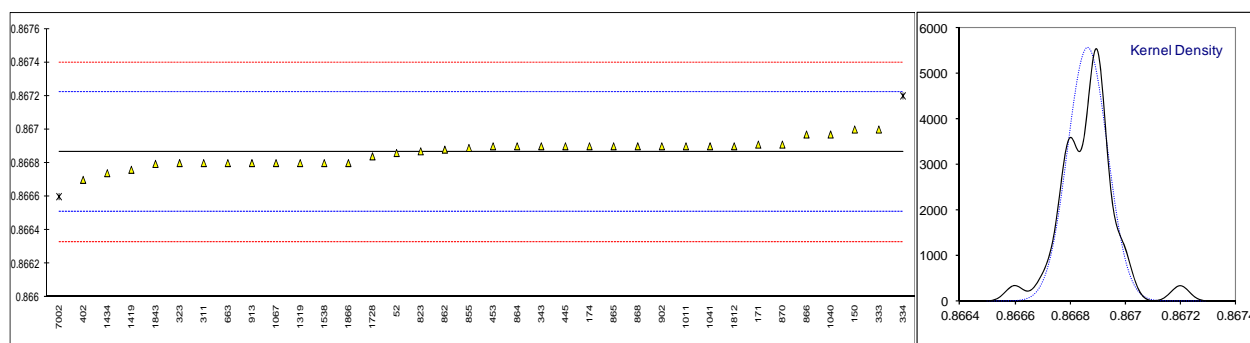


Determination of Copper Corrosion on Toluene sample #15014

lab	method	value	mark	z(targ)	remarks
52	D849	1A		----	
150	D130	1A		----	
171	D849	1		----	
174	D849	1A		----	
311	D849	1A		----	
323	D849	1A		----	
333	D849	1		----	
334		----		----	
343	D849	1A		----	
402		----		----	
445	D849	1		----	
453		----		----	
551		----		----	
555		----		----	
663	D849	1A		----	
823	D849	1A		----	
855	D849	1A		----	
862	D849	1A		----	
864	D849	1A		----	
865		1A		----	
866	D849	1A		----	
868	D849	1A		----	
870	D849	1A		----	
902		----		----	
912		----		----	
913	D849	1A		----	
1011	D849	1A		----	
1040	ISO2160	1		----	
1041		----		----	
1067	D849	1A		----	
1151		----		----	
1319	D849	1A		----	
1419		----		----	
1434	D849	1A		----	
1538		----		----	
1728	D849	1A		----	
1812		----		----	
1843		----		----	
1866		----		----	
7002		----		----	
	normality	n.a.			
	n	25			
	outliers	n.a.			
	mean (n)	1 (1A)			
	st.dev. (n)	n.a.			
	R(calc.)	n.a.			
	R(D849:11)	unknown			

Determination of Density at 20°C on Toluene sample #15014: results in kg/L

lab	method	value	mark	z(targ)	remarks
52	D4052	0.86686		-0.03	
150	ISO12185	0.8670		0.76	
171	D4052	0.86691		0.25	
174	D4052	0.8669		0.20	
311	D4052	0.8668		-0.36	
323	D4052	0.8668		-0.36	
333	ISO12185	0.8670		0.76	
334	ISO12185	0.8672	R(0.05)	1.88	
343	D4052	0.8669		0.20	
402	ISO12185	0.8667		-0.92	
445	D4052	0.8669		0.20	
453	D4052	0.8669		0.20	
551		----		----	
555		----		----	
663	D4052	0.8668		-0.36	
823	ISO12185	0.86687		0.03	
855	D4052	0.86689		0.14	
862	D4052	0.86688		0.09	
864	D4052	0.8669		0.20	
865	D4052	0.8669		0.20	
866	D4052	0.86697		0.59	
868	D4052	0.86690		0.20	
870	D4052	0.86691		0.25	
902	D4052	0.8669		0.20	
912		----		----	
913	D4052	0.8668		-0.36	
1011	D4052	0.8669		0.20	
1040	ISO12185	0.86697		0.59	
1041	ISO12185	0.86690	C	0.20	first reported: 866.90
1067	D4052	0.8668		-0.36	
1151		----		----	
1319	ISO12185	0.8668		-0.36	
1419	ISO12185	0.86676	C	-0.59	first reported: 866.76
1434	D4052	0.86674		-0.70	
1538	ISO12185	0.8668		-0.36	
1728	ISO12185	0.86684		-0.14	
1812	ISO12185	0.8669	C	0.20	first reported: 0.8789
1843	D4052	0.866795		-0.39	
1866	ISO12185	0.8668		-0.36	
7002	in house	0.8666	R(0.05)	-1.48	
normality		OK			
n		34			
outliers		2			
mean (n)		0.86686			
st.dev. (n)		0.000072			
R(calc.)		0.00020			
R(D4052:02e1)		0.00050			



Determination of Distillation on Toluene sample #15014; results in °C

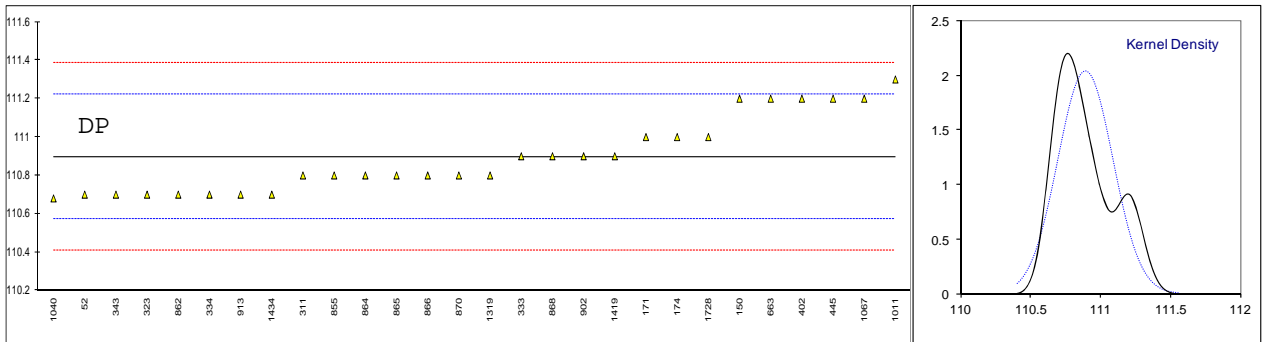
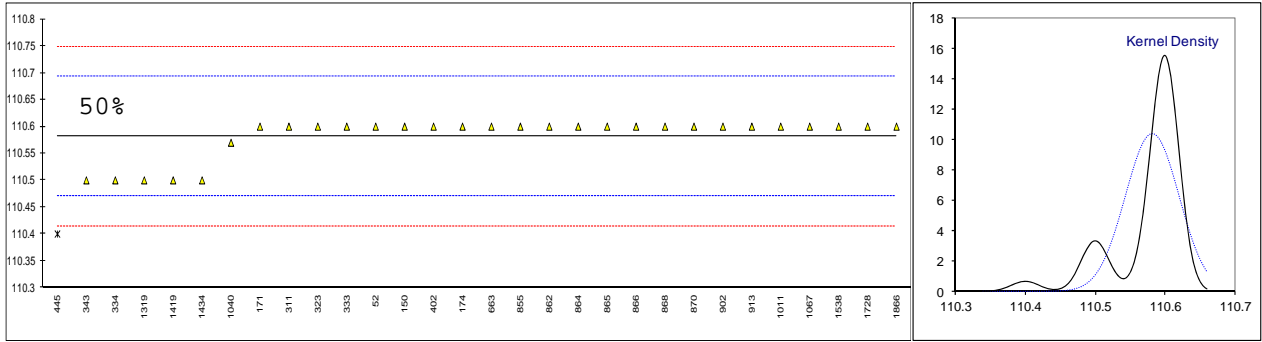
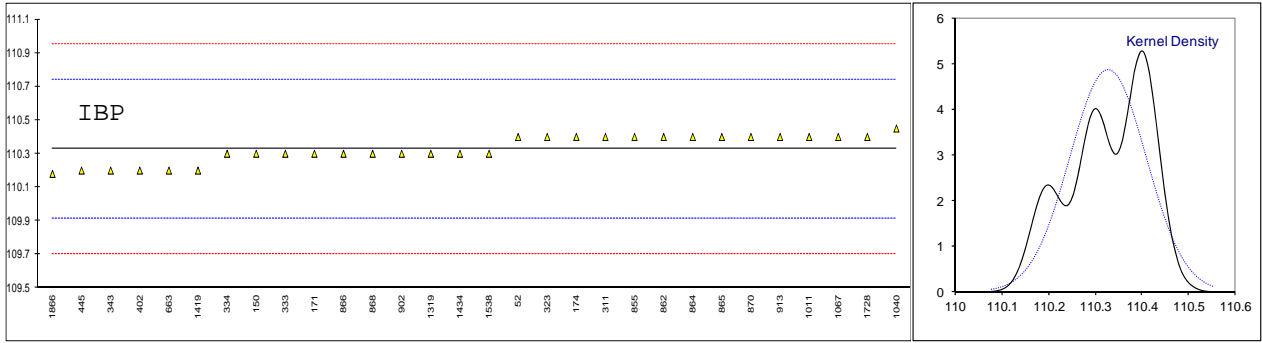
lab		mode	IBP	mark	z(tar g)	50%	mark	z(targ)	DP	mark	z(targ)
52	D850	Automated	110.4		0.35	110.6		0.33	110.7		-1.20
150	D850	Automated	110.3		-0.13	110.6		0.33	111.2		1.87
171	D850	Automated	110.3		-0.13	110.6		0.33	111.0		0.64
174	D850	Automated	110.4		0.35	110.6		0.33	111.0		0.64
311	D850	Automated	110.4		0.35	110.6		0.33	110.8		-0.59
323	D850	Manual	110.4		0.35	110.6		0.33	110.7		-1.20
333	D850	Automated	110.3		-0.13	110.6		0.33	110.9		0.03
334	D850	Automated	110.3	C	-0.13	110.5		-1.47	110.7		-1.20
343	D850	Automated	110.2	C	-0.62	110.5		-1.47	110.7		-1.20
402	D850	Manual	110.2		-0.62	110.6		0.33	111.2		1.87
445	D850	Manual	110.2		-0.62	110.4	R(0.01)	-3.26	111.2		1.87
453		----	----		----	----		----	----		----
551		----	----		----	----		----	----		----
555		----	----		----	----		----	----		----
663	D850	Automated	110.2		-0.62	110.6		0.33	111.2		1.87
823		----	----		----	----		----	----		----
855	D850	Manual	110.4		0.35	110.6		0.33	110.8		-0.59
862	D850	Manual	110.4		0.35	110.6		0.33	110.7		-1.20
864	D850	Manual	110.4		0.35	110.6		0.33	110.8		-0.59
865	D850	Manual	110.4		0.35	110.6		0.33	110.8		-0.59
866	D850	Manual	110.3		-0.13	110.6		0.33	110.8		-0.59
868	D850	Manual	110.3		-0.13	110.6		0.33	110.9		0.03
870	D850	Manual	110.4		0.35	110.6		0.33	110.8		-0.59
902	D850	Manual	110.3		-0.13	110.6		0.33	110.9		0.03
912		----	----		----	----		----	----		----
913	D850	Manual	110.4		0.35	110.6		0.33	110.7		-1.20
1011	D850	Automated	110.4		0.35	110.6		0.33	111.3		2.48
1040	DIN51761	Manual	110.45		0.59	110.57		-0.21	110.68		-1.32
1041		----	----		----	----		----	----		----
1067	D850	Manual	110.4		0.35	110.6		0.33	111.2		1.87
1151		----	----		----	----		----	----		----
1319	D850	Manual	110.3		-0.13	110.5		-1.47	110.8		-0.59
1419	D850	Automated	110.2		-0.62	110.5		-1.47	110.9		0.03
1434	D850	Automated	110.3		-0.13	110.5		-1.47	110.7		-1.20
1538	D850	Automated	110.3		-0.13	110.6		0.33	----		----
1728	D850	Manual	110.4		0.35	110.6		0.33	111.0		0.64
1812		----	----		----	----		----	----		----
1843		----	----		----	----		----	----		----
1866	D850	Automated	110.18		-0.71	110.60		0.33	----		----
7002		----	----		----	----		----	----		----
	normality	Autom./Man.	OK			suspect			OK		
	n	14/16	30			29			28		
	outliers		0			1			0		
	mean (n)		110.33			110.58			110.90		
	st.dev. (n)		0.082			0.038			0.196		
	R(calc.)		0.23			0.11			0.55		
	R(D850:11)		0.58			0.16			0.46		

Both laboratories 334 and 343 first reported for Initial Boiling Point: 109.7

Theoretical mid boiling point = 110.6°C

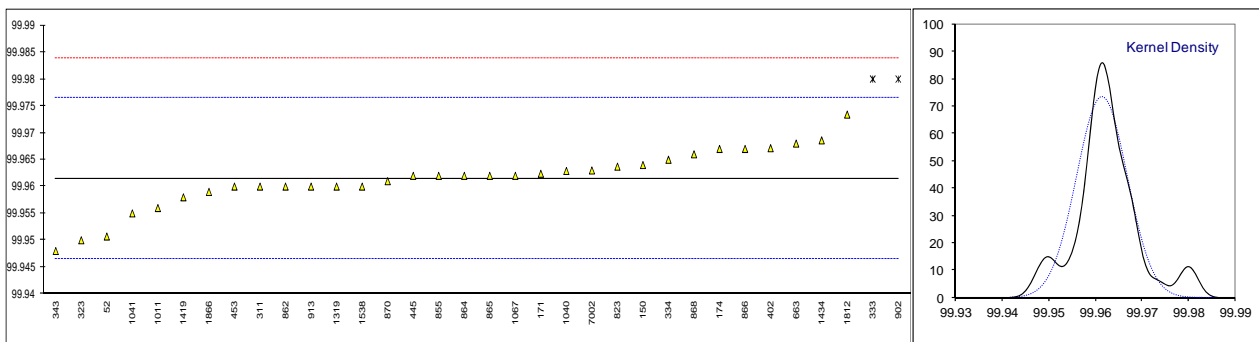
After manual correction:

445	D850	Manual	110.4	0.32	110.6	0.32	111.4	3.05
	normality		OK		suspect		OK	
	n		30		30		28	
	outliers		0		0		0	
	mean (n)		110.33		110.58		110.90	
	st.dev. (n)		0.079		0.038		0.211	
	R(calc.)		0.22		0.11		0.59	
	R(D850:11)		0.58		0.16		0.46	



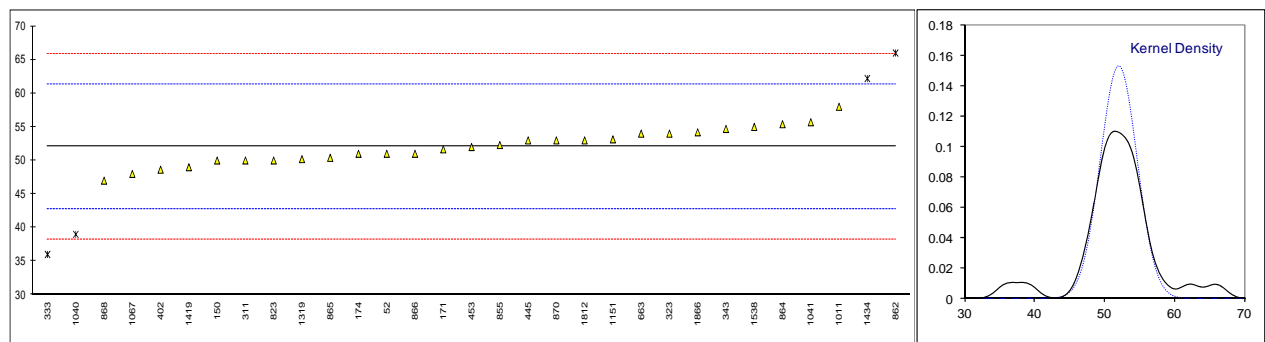
Determination of Purity on Toluene sample #15014; results in %M/M

lab	method	value	mark	z(targ)	remarks
52	D7504	99.9507		-1.43	
150	D2360	99.964		0.34	
171	D2360	99.96238		0.13	
174	D2360	99.967		0.74	
311	D2360	99.96		-0.19	
323	D2360	99.95		-1.53	
333	D2360	99.98	DG(0.05)	2.47	
334	D2360	99.965		0.47	
343	D2360	99.948		-1.79	
402	D2360	99.96714		0.76	
445	D6526	99.962		0.07	
453	D2360	99.96		-0.19	
551		----		----	
555		----		----	
663	D2360	99.968		0.87	
823	D2360	99.9637		0.30	
855	D2360	99.962		0.07	
862	D2360	99.960		-0.19	
864	D7504	99.962		0.07	
865	D7504	99.962		0.07	
866	D2360	99.967		0.74	
868	D2360	99.966		0.61	
870	D2360	99.961		-0.06	
902	INH-135	99.98	DG(0.05)	2.47	
912		----		----	
913	D2360	99.96		-0.19	
1011	D2360	99.956		-0.73	
1040	D2360	99.9629		0.19	
1041	D2360	99.955		-0.86	
1067	in house	99.962		0.07	
1151		----		----	
1319	D2360	99.96		-0.19	
1419	D6526	99.958		-0.46	
1434	D2360	99.9686		0.95	
1538	D2360	99.96		-0.19	
1728		----		----	
1812	D2360	99.9734		1.59	
1843		----		----	
1866	D2360	99.959		-0.33	
7002	D2360	99.963		0.21	
normality		OK			
n		32			
outliers		2			
mean (n)		99.9614			
st.dev. (n)		0.00542			
R(calc.)		0.0152			
R(D2360:11)		0.0210			



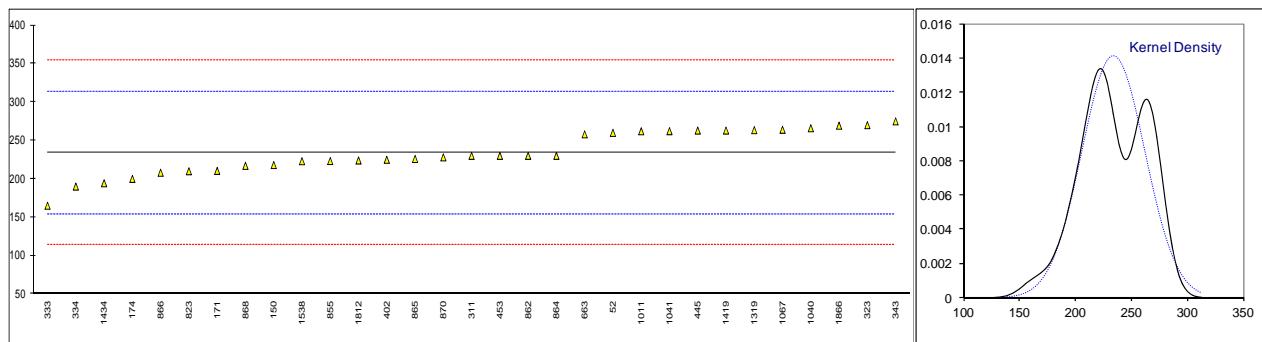
Determination of Benzene on Toluene sample #15014; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7504	51	C	-0.23	first reported: 0.0051
150	D2360	50		-0.45	
171	D2360	51.6536		-0.09	
174	D2360	51		-0.23	
311	D2360	50		-0.45	
323	D2360	54		0.42	
333	D2360	36	R(0.01)	-3.49	
334		----		----	
343	D2360	54.7		0.58	
402	D2360	48.63		-0.74	
445	D6526	53		0.21	
453	D2360	52		-0.01	
551		----		----	
555		----		----	
663	D2360	54		0.42	
823	D2360	50		-0.45	
855	D2360	52.3		0.05	
862	D2360	66	R(0.01)	3.04	
864	D7504	55.4		0.73	
865	D7504	50.4		-0.36	
866	D2360	51		-0.23	
868	D2360	47		-1.10	
870	D2360	53	C	0.21	first reported: 73
902		----		----	
912		----		----	
913		----		----	
1011	D2360	58		1.30	
1040	D2360	39	R(0.01)	-2.84	
1041		55.7		0.79	
1067	in house	48		-0.88	
1151	in house	53.15		0.24	
1319	D2360	50.2		-0.40	
1419	D6526	49		-0.66	
1434	D2360	62.2	R(0.05)	2.21	
1538	D2360	55		0.64	
1728		----		----	
1812		53		0.21	
1843		----		----	
1866	D2360	54.2		0.47	
7002		----		----	
	normality	OK			
	n	27			
	outliers	4			
	mean (n)	52.05			
	st.dev. (n)	2.609			
	R(calc.)	7.31			
	R(Horwitz)	12.86			



Determination of Nonaromatics on Toluene sample #15014; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7504	260	C	0.65	
150	D2360	218		-0.40	
171	D2360	210.3989		-0.59	
174	D2360	200		-0.85	
311	D2360	230		-0.10	
323	D2360	270		0.90	
333	D2360	165		-1.73	
334	D2360	190	C	-1.10	
343	D2360	274.9		1.02	
402	D2360	224.89		-0.23	
445	D6526	263		0.72	
453	D2360	230		-0.10	
551		----		----	
555		----		----	
663	D2360	258		0.60	
823	D2360	210		-0.60	
855	D2360	223.2		-0.27	
862	D2360	230		-0.10	
864	D7504	230		-0.10	
865	D7504	226		-0.20	
866	D2360	208		-0.65	
868	D2360	217		-0.43	
870	D2360	228		-0.15	
902		----		----	
912		----		----	
913		----		----	
1011	D2360	262		0.70	
1040	D2360	266		0.80	
1041	D2360	262.17		0.70	
1067	in house	264		0.75	
1151		----		----	
1319	D2360	263.5		0.73	
1419	D6526	263		0.72	
1434	D2360	194.3		-1.00	
1538	D2360	223		-0.28	
1728		----		----	
1812	D2360	224		-0.25	
1843		----		----	
1866	D2360	269.3		0.88	
7002		----		----	
normality		OK			
n		31			
outliers		0			
mean (n)		234.12			
st.dev. (n)		28.218			
R(calc.)		79.01			
R(D2360:11)		111.97			



APPENDIX 2

Number of participants in the Benzene PT

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

Number of participants in the Toluene PT

1 lab in AUSTRALIA
1 lab in BELGIUM
2 labs in BRAZIL
1 lab in CANADA
7 labs in CHINA, People's Republic
2 labs in FRANCE
3 labs in GERMANY
2 labs in INDIA
1 lab in IRAN, Islamic Republic of
1 lab in ISRAEL
1 lab in JAPAN
2 labs in NETHERLANDS
1 lab in POLAND
1 lab in PORTUGAL
2 labs in ROMANIA
2 labs in SAUDI ARABIA
1 lab in SLOVAKIA
1 lab in SOUTH KOREA
1 lab in SPAIN
1 lab in THAILAND
1 lab in TURKEY
2 labs in UNITED KINGDOM
3 labs in UNITED STATES OF AMERICA

APPENDIX 3

Abbreviations:

C	= final 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's outlier test
R(0.05)	= straggler in Rosner's outlier test
fr	= first reported
E	= error in calculations
ex	= excluded from calculations
n.a.	= not applicable
fr	= first reported
U	= reported in different unit
SDS	= Safety Data Sheet

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