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# Validation for the transition of SPSS QI Analyst to the SPC for Excel program for quality control charting

Inorganic Geochemistry, Centre for Environmental Geochemistry

Commissioned Report CR/18/044N



# Validation for the transition of SPSS QI Analyst to the SPC for Excel program for quality control charting

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# Foreword

This document reports the validation of new quality control software for use in the Inorganic Geochemistry Facility. The project conducted involved compiling datasets to provide evidence to the reproducible capabilities between two control-charting programs. The reproducibility of the functions in SPC for Excel (version 5, 2017) with existing software (SPSS QI Analyst version 3.5, 1998 (QIA)) was confirmed which allows the use of SPC for Excel within the [Inorganic Geochemistry](#) UKAS ISO 17025 accreditation framework - .

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# Glossary

QC	Quality control check sample. A sample used for monitoring day-to-day, batch-to-batch or overall analytical performance. QC samples are usually sufficiently stable and obtainable in sufficient quantities as to be available for analysis over an extended period.
SD	Standard deviation
USL and LSL	Upper and lower specification limits. Quantity defining an interval about the result of a measurement expected to encompass a large fraction of the distribution of values that could be attributed to the measurand.
UCL and LCL	Upper and lower control limits ( $\bar{x} \pm 3SL$ )
UWL and LWL	Upper and lower warning limits ( $\bar{x} \pm 2SL$ )
CL	Centreline – the target value



# Summary

The statistical process control charting software utilised by the Inorganic Geochemistry team, SPSS QI Analyst version 3.5, (1998, (QIA)), was no longer viable because it was incompatible with operating system requirements for networked computers. Therefore, an alternative program, SPC for Excel version 5, (2017, (SPC)), has been validated to replace the legacy version of QIA.

The benefits of using SPC include but are not limited to the following:

- Conformity with accredited QC processes according to the Inorganic Geochemistry Analytical Quality Control Operating Procedure (AGN 1.7)
- Ease of transferring results from the analytical software
- Program is accessible to computers connected to the network
- Control charting and recording QC checks are all accomplished using Excel alone
- User friendly with moderate Excel skills
- Lower cost per licence than the latest version of the existing software

The following document provides evidence to satisfy the requirements of UKAS accredited Standard ISO17025 by validating the new software system against the existing QIA software according to a validation plan using two complementary approaches. Specifically, this validation document comprises:

- Tests with a synthetic dataset, which confirms that QIA and SPC for Excel produce the same result against the criteria specified by Analytical Quality Control procedures (AGN 1.7)
- Tests with standards run during a recent large stream water analysis programme, which confirms that QIA and SPC for Excel control charts are able to perform the same quality control checks for analytes in “real” control sample data
- A comparative table of terminology differences between QIA and SPC for Excel

A companion document “SPC for Excel Instruction manual v2\_WORKING VERSION”, provides working guidance on the operation of SPC for Excel version 5 2017, located in *Appendix 5*.

# 1 Introduction

A validation plan strategy using (1) synthetic data and, (2) a recent dataset associated with a large analysis programme, was devised to provide robust evidence for the transition.

An artificially generated dataset was created to easily compare and demonstrate both control charting programs for similarities and discrepancies under controlled conditions.

This approach was followed by an assessment of SPC for Excel against QIA using a more constrained set of real control sample data from a recent large programme of stream water analyses being conducted in Inorganic Geochemistry to demonstrate its functionality in real situations. Stream water samples fall within the scope of the Inorganic Geochemistry (IG) UKAS accreditation and are a major analytical matrix across the IG laboratories.

## 1.1 INDIVIDUAL LEVEY-JENNINGS CONTROL CHART

Levey-Jennings control charts are used to monitor the performance of individual QC results in real time. The Levey-Jennings charts otherwise known as an individual control chart has six types of boundaries namely the USL, LSL, UCL, LCL, UWL, and LWL as defined in section 4.1. Depending on where a given point resides within these boundaries at any given time defines whether the point is deemed in control or out of control, which conforms to Analytical Quality Control procedure (AGN 1.7 detailed in section 2.1).

A randomly generated data set ( $N=100$ , Average=1.000, Std dev=0.100) was used for the construction of the charts for the purposes of demonstrating the capabilities and reproducibility between the SPC for Excel and QIA software, with no failures arising in the first instance (i.e. demonstrating software performance under the best case analytical scenario).

This then allows the manipulation of this manageable dataset to highlight the reproducibility between QIA and SPC for Excel regarding the plotting control limits and identifying rule violations.

## **1.2 BATCH MEAN MEASUREMENT CHARTS (BMMC)**

Batch Mean Measurement Charts (BMMC) are plotted based on the average QC result of a batch from a single analytical run. They are used to identify potential deterioration in performance of the method as described in Analytical Quality Control Procedures (AGN 1.7), which should identify potential trends which signal possible deterioration in performance as specified in section 2.2.

Similar to the proof of reproducibility for the Levey-Jennings individuals control charts, a synthetic dataset was constructed to prove the reproducibility between QIA and SPC for Excel. Firstly, the format of the synthetic dataset for SPC for Excel was arranged in a table array using MS Excel Pivot Tables (Appendix 5), this was done to allow SPC for Excel to correctly identify subgroups based on run dates, as specified in Analytical Quality Control Procedures (AGN 1.7). In QIA this process is undertaken automatically by the software, whilst it is user driven in Excel/SPC.

## 2 Validation of SPC using synthetic data

### 2.1 INDIVIDUAL CONTROL CHART DATA AND RESULTS

Using both programs to construct normally distributed points within a Levey-Jennings control chart, the randomly generated dataset, with no rule violations, was plotted as shown in Figure 1 and Figure 2. The dataset used to construct the control chart is shown in Appendix 1.

The normally distributed dataset was further edited to produce three additional sets of results to demonstrate failures that could arise from the control chart based on an Analytical Quality Control procedure (AGN 1.7). These results are shown in Appendix 1, with the edited data values highlighted. Figure 3 to Figure 8 display the charts from both programs comparing graph display, points plotted, and boundaries set.

These augmentations display rule violations are specified in an Analytical Quality Control Procedure (AGN 1.7 section 13):

- i. 1 point away from the specified limits
- ii. 1 point away from 3 standard deviations (SD) from the mean
- iii. 2 of 2 consecutive points away from 2 SD from the mean

Figure 3 and Figure 4 display point 1 with a converted value to be above the specified limit. Figure 5 and Figure 6 display the value for point 1 to be above 3 SD from the mean but within the specified limits. Lastly, Figure 7 and Figure 8 were made by converting the value for points 1 and 2 to be outside 2 SD from one side of the mean. The control charting program, subsequently highlights the point associated with a test rule violation as red.

The exact values for the limits from each chart constructed in SPC for Excel (Figure 1, Figure 3, Figure 5, Figure 7) and the limits from each chart constructed in QI Analyst (Figure 2, Figure 4, Figure 6, Figure 8) are summarised in Table 1.

Table 1 proves that using a synthetic dataset displaying, both QIA and SPC for Excel have the same average, warning limits, and control limits for normally distributed points and the forced test rule violations on the control charts.

Table 2 summarises the differences for how test rule violations are highlighted between the SPC for Excel and the QIA program. For 2 of 2 consecutive points outside 2 SD away from the mean, on SPC for Excel both points are highlighted red. However, on QIA only the 2nd of 2 consecutive points is highlighted red, with subsequent 2 of 2 consecutive points outside 2 SD. Additionally, points which

are outside the specified limits, and within control limits can only be manually highlighted red by the analyst on SPC for Excel.

## 2.2 BMMC CONTROL CHART DATA AND RESULTS

The BMMC control chart utilised by both QIA and SPC for Excel are XBar-R charts as displayed in Figure 9 and Figure 10. The initial BMMC synthetic dataset was further augmented to allow rule violations associated with BMMC to be observed. Two trends observed in BMMC control charts which are classified as test rule violations stated in an Analytical Quality Control Procedure (AGN 1.7 section 14) are as follows:

- i. 8 consecutive points successively rising or falling
- ii. 10 of 11 consecutive points above or below the mean

These rule violations were tested with a synthetic dataset for both QIA and SPC for Excel to prove the reproducibility of the constructed BMMC control charts. The synthetic dataset utilised to display these rule violations are located in Appendix 1. Figure 11 and Figure 12 display control charts highlighting the test rule violation of 10 of 11 consecutive points above the mean for both programs. Figure 13 and Figure 14 display control charts highlighting the test rule violation of 8 consecutive points rising progressively for both SPC for Excel and QIA programs respectively. The averaged centreline on the BMMC chart for both programs are identical. However, there is a difference to the calculation of the limits between both programs as shown in Table 3.

Table 4 item 1 explains the discrepancy in the calculation of control limits.

Table 4 item 2 explains a slight difference in how both programs handle average calculations of disabled points. Subsequent discussions made in

Table 4 detail differences in how test rule violations are presented by the charts.

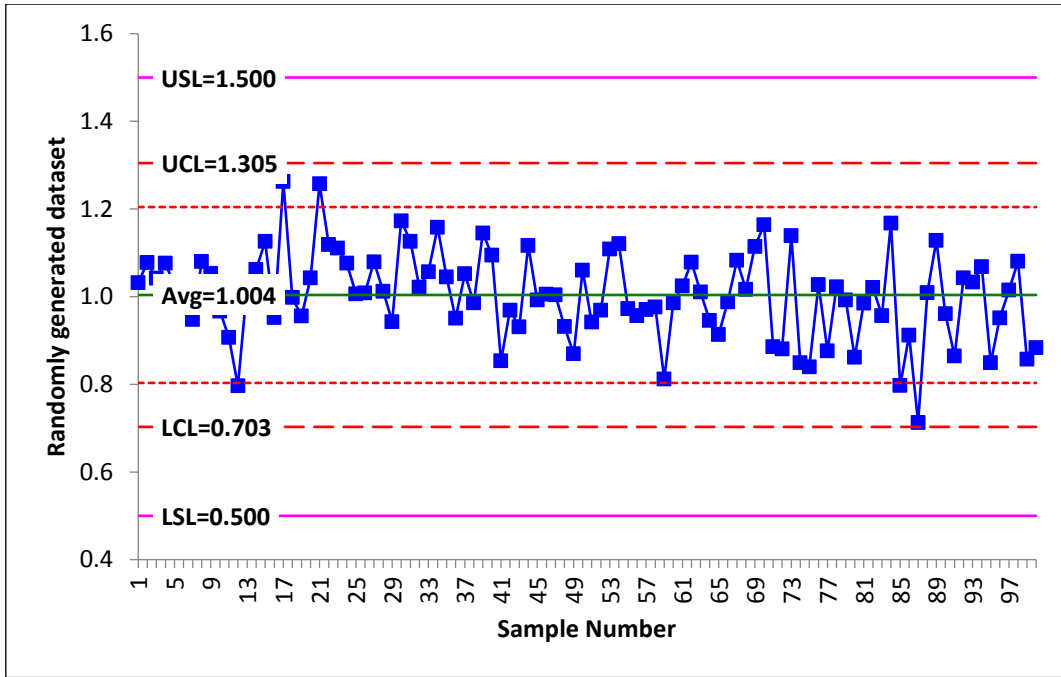


Figure 1. Normal distribution of randomly generated dataset from SPC for Excel.

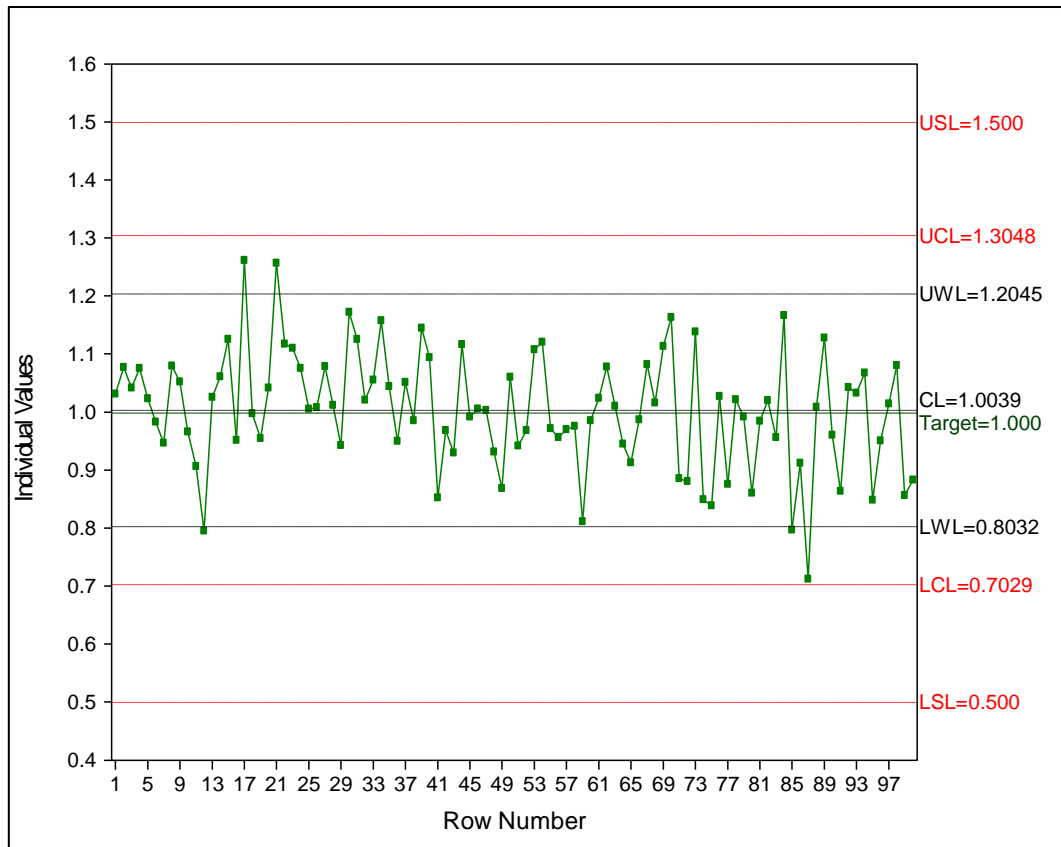


Figure 2. Normal distribution of randomly generated dataset from QIA.

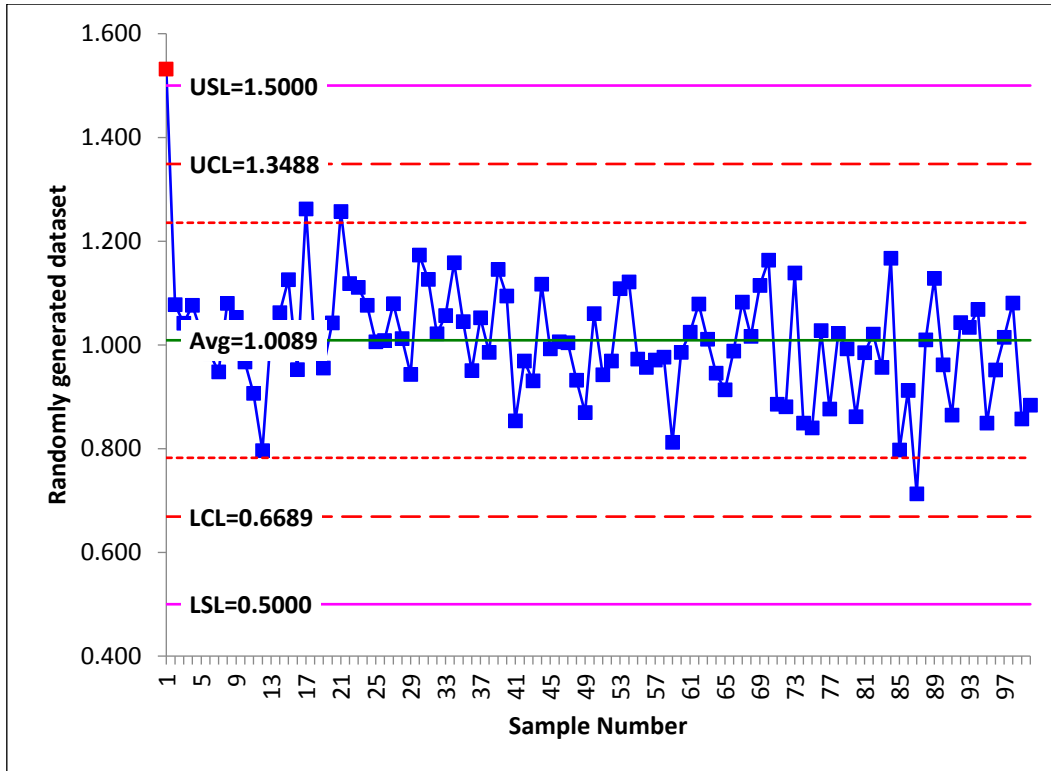


Figure 3. 1 point away from the specified limit from SPC for Excel.

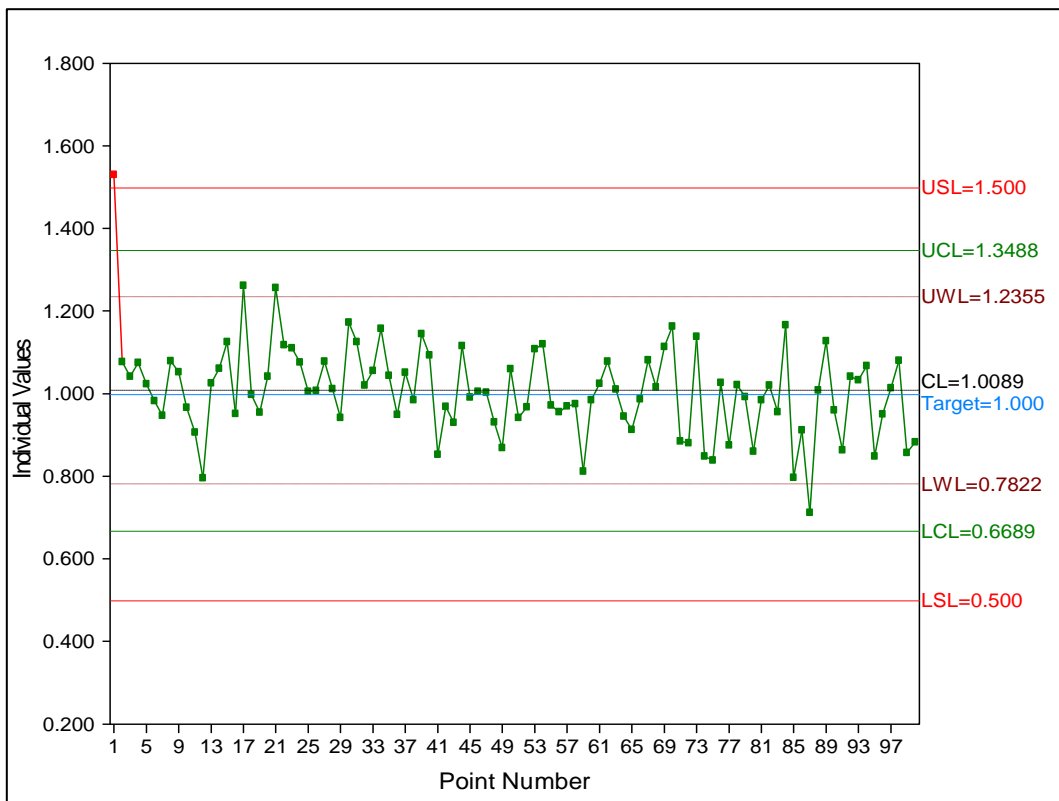


Figure 4. 1 point away from the specified limit from QIA.

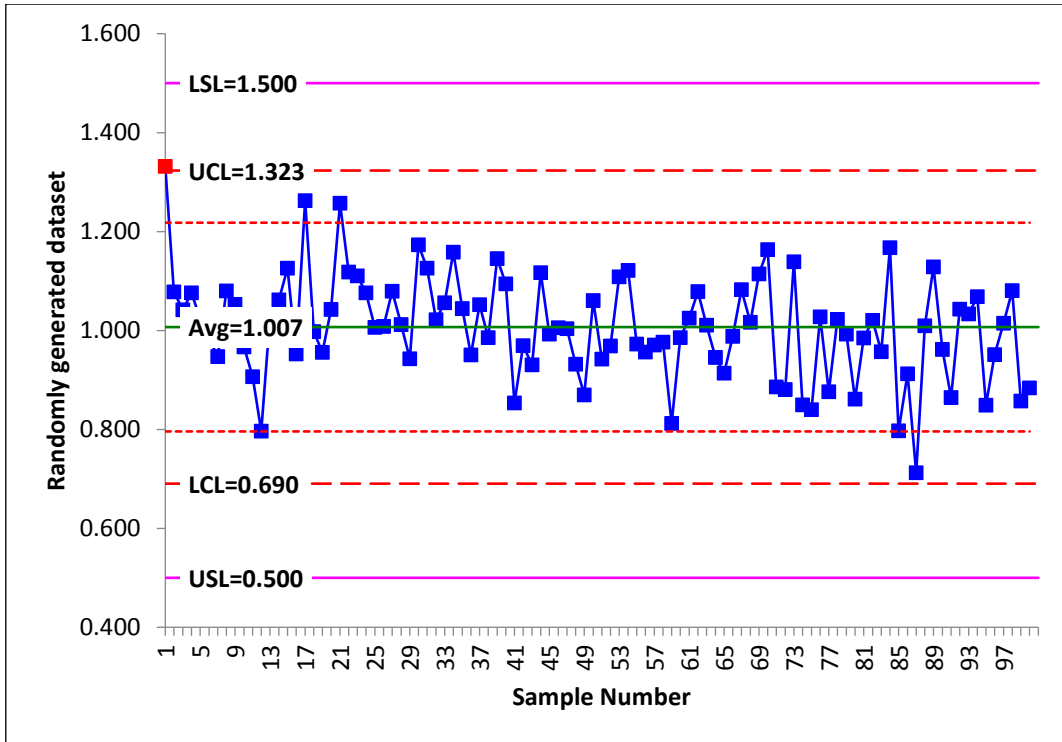


Figure 5. 1 point away 3 SD from the mean from SPC for Excel.

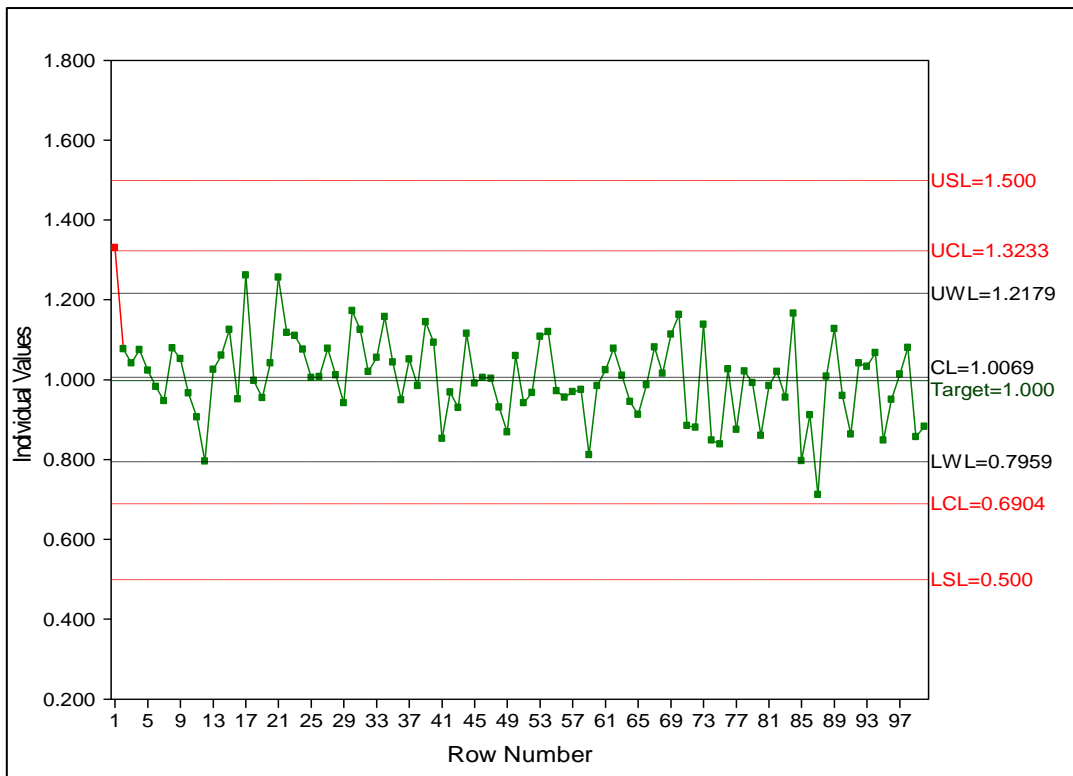


Figure 6. 1 point away 3 SD from the mean from QIA.



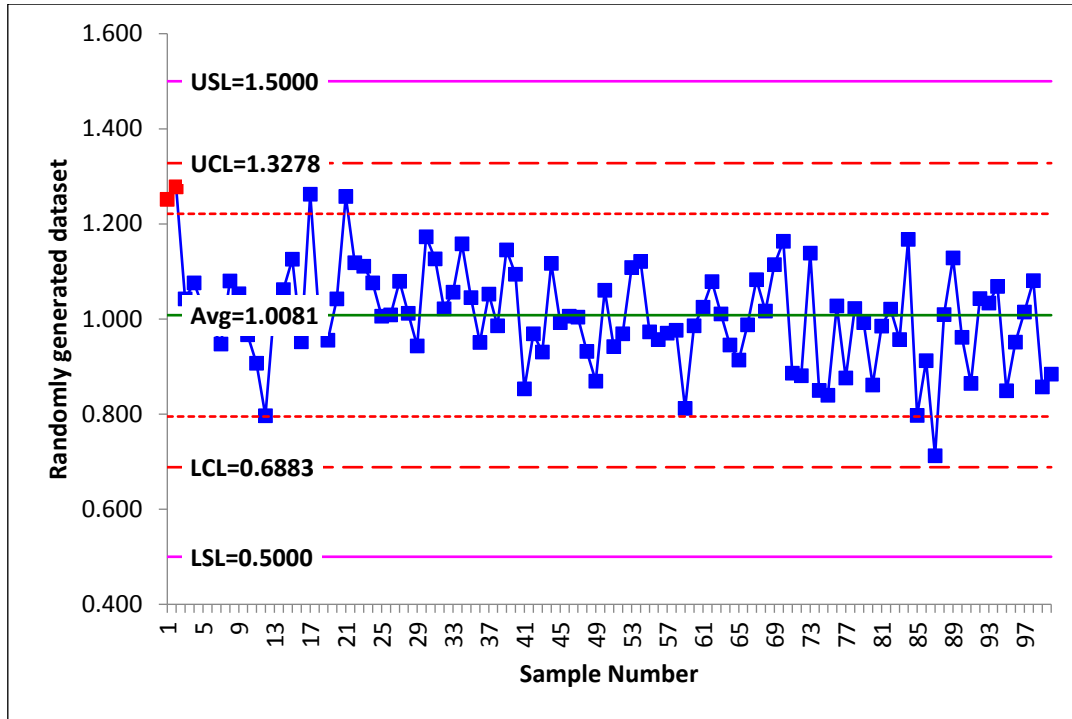


Figure 7. 2 of 2 consecutive points away 2 SD from the mean from SPC for Excel.

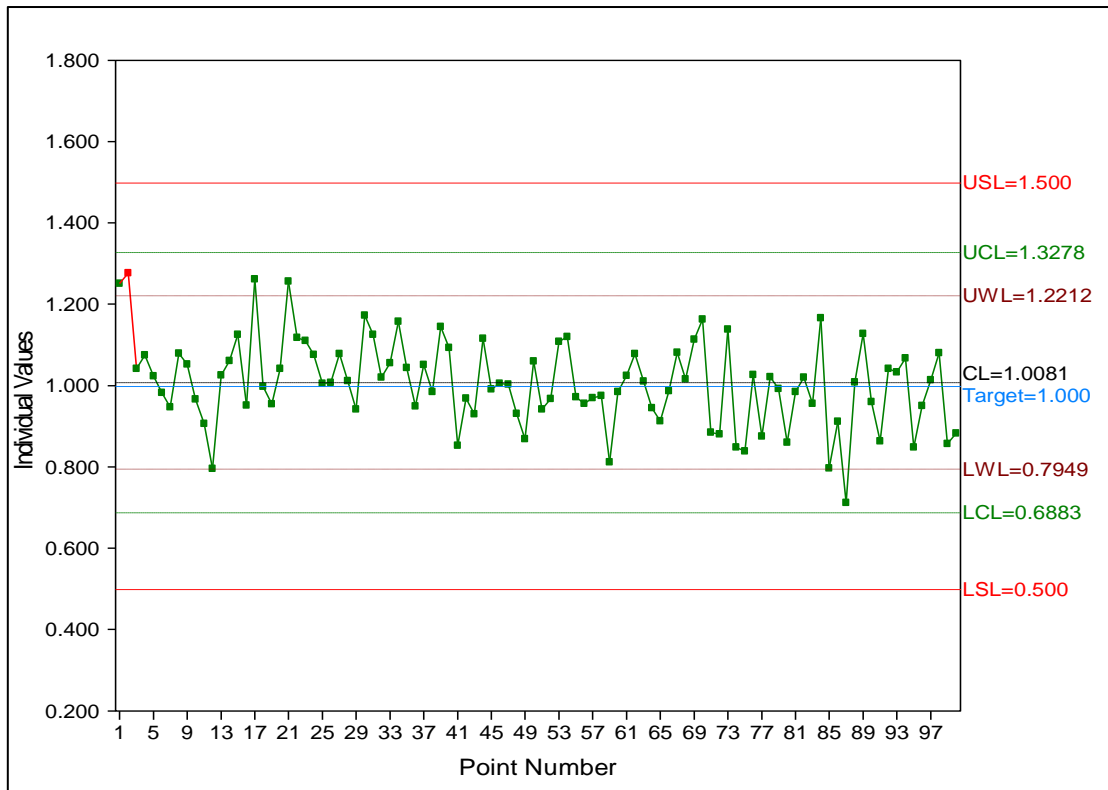


Figure 8. 2 of 2 consecutive points away 2 SD from the mean from QIA.

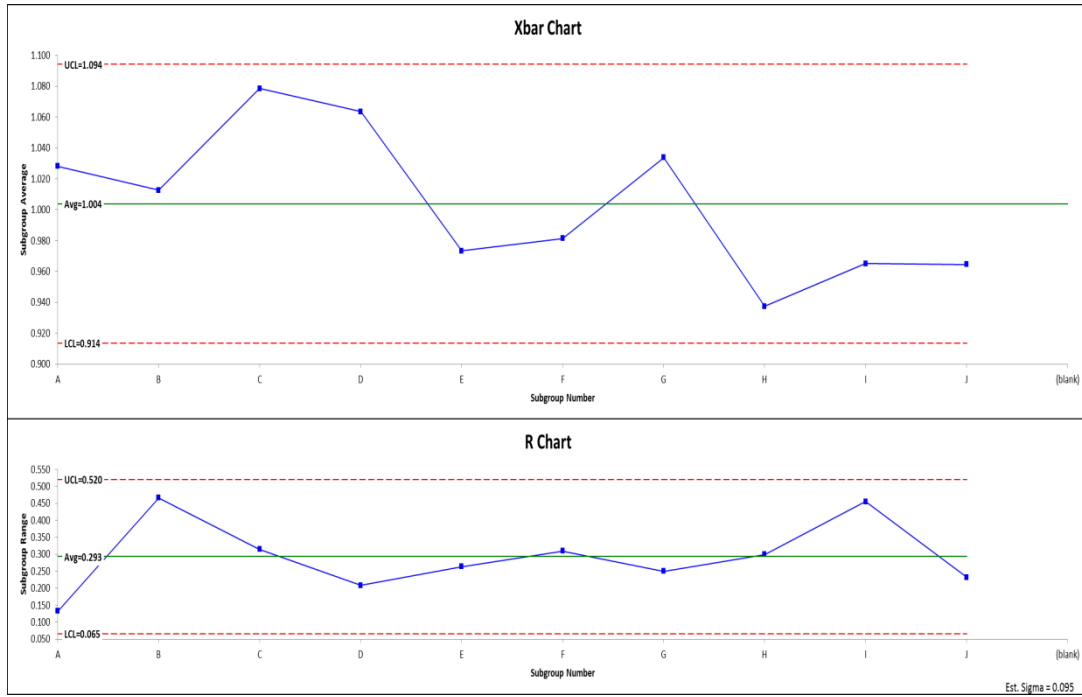


Figure 9. SPC for Excel Xbar R-chart constructed using randomly generated dataset.

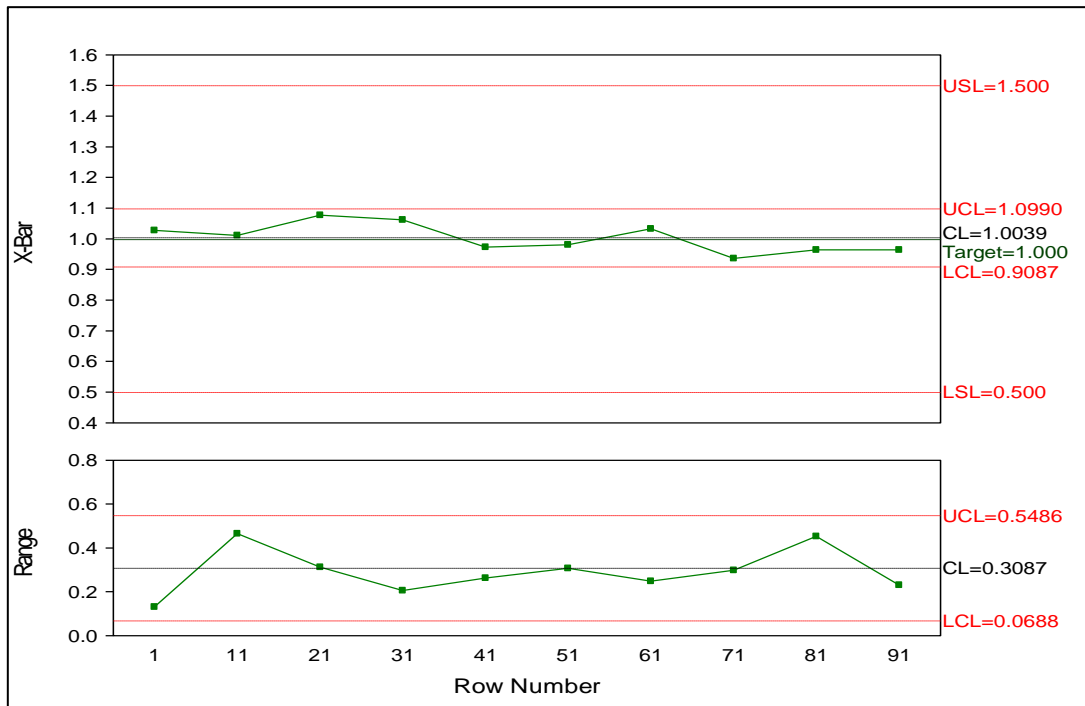


Figure 10. QIA Xbar R-chart constructed using randomly generated dataset.

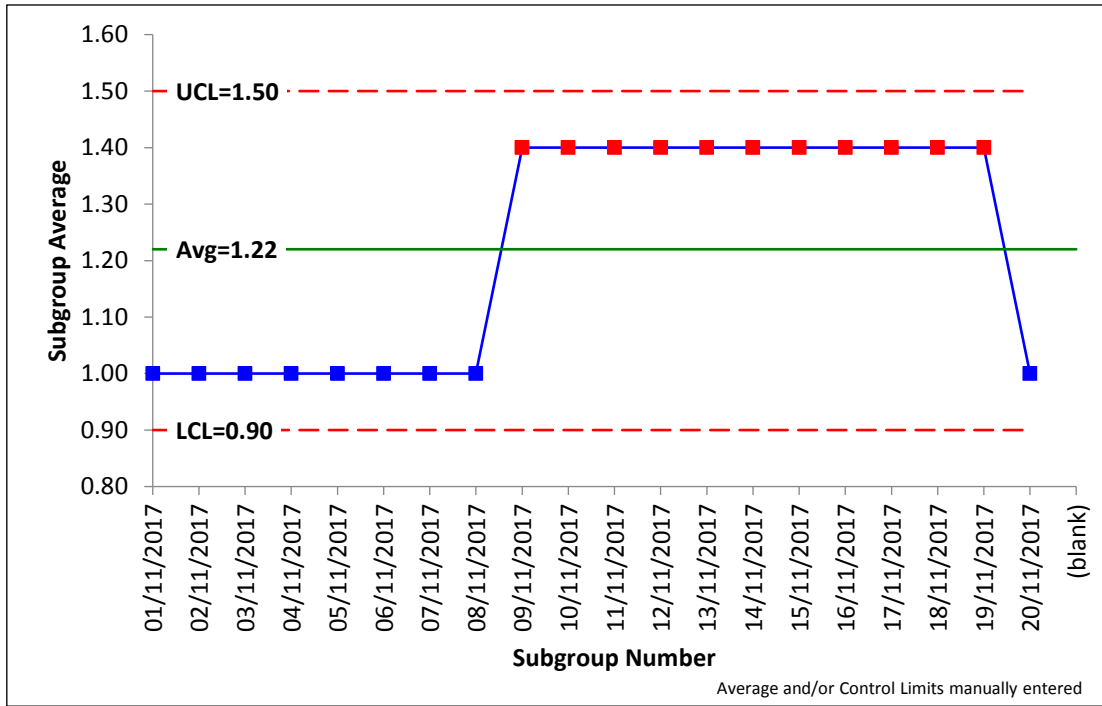


Figure 11. SPC for Excel control chart displaying 10 of 11 above mean violation.

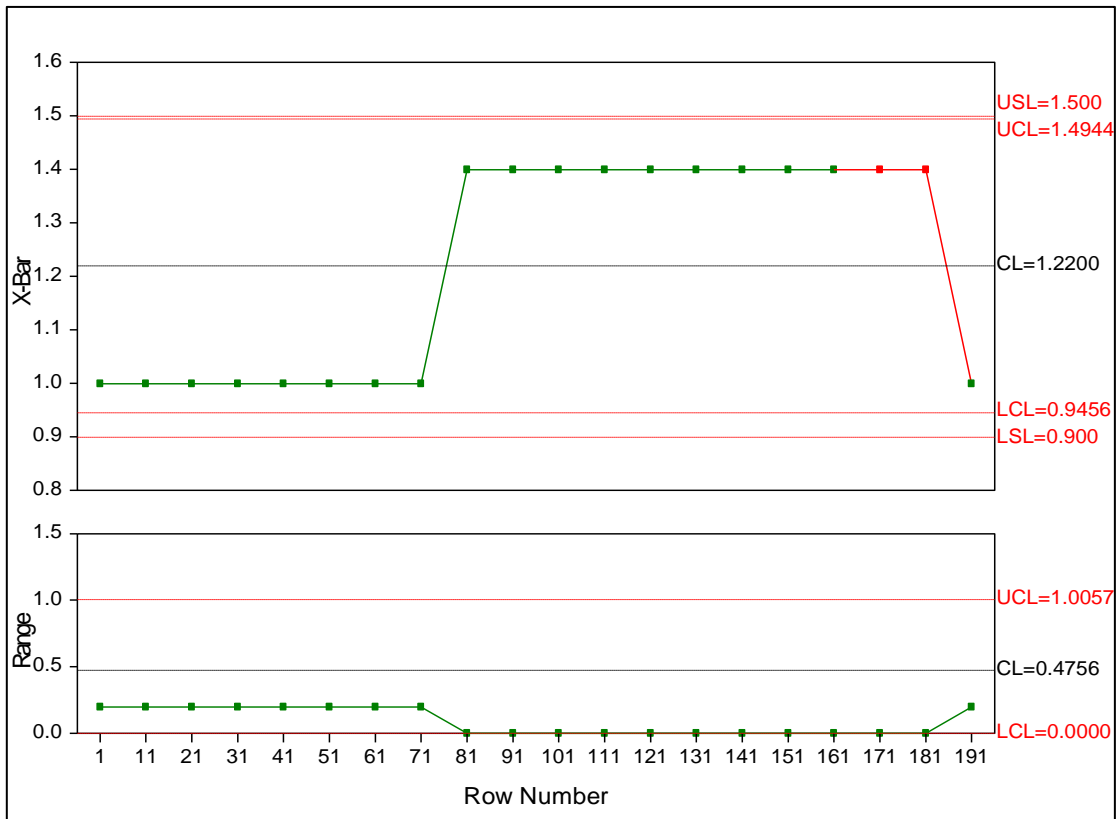


Figure 12. QIA control chart displaying 10 of 11 above mean violation.

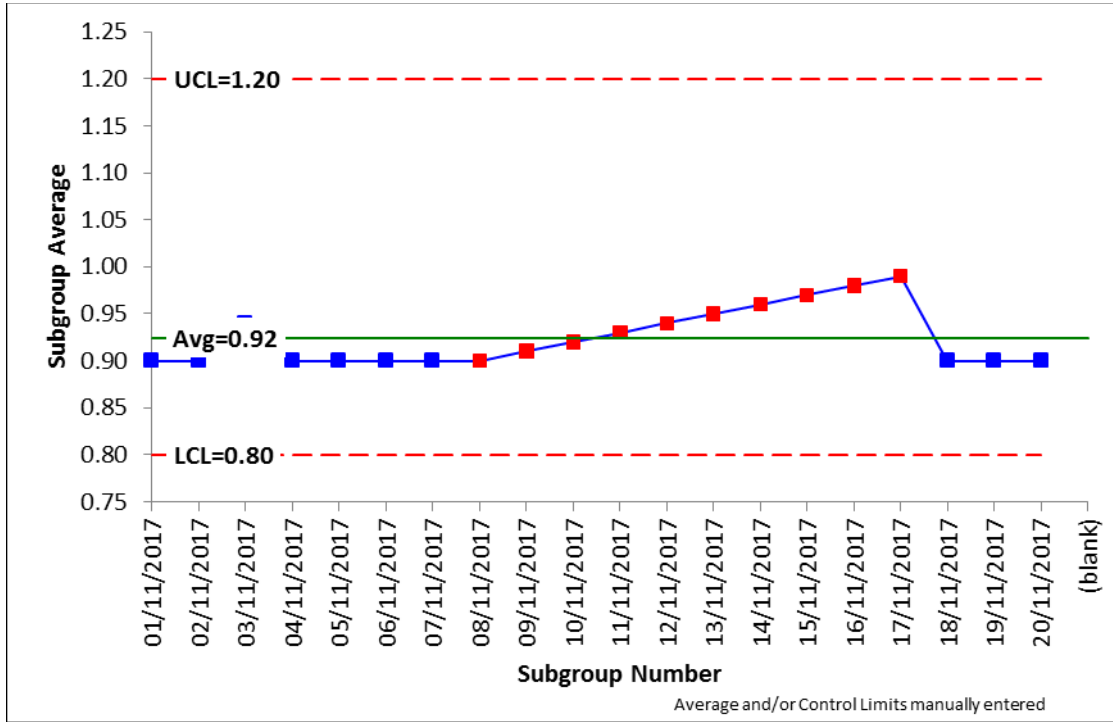


Figure 13. SPC for Excel control chart displaying 8 consecutive points rising.

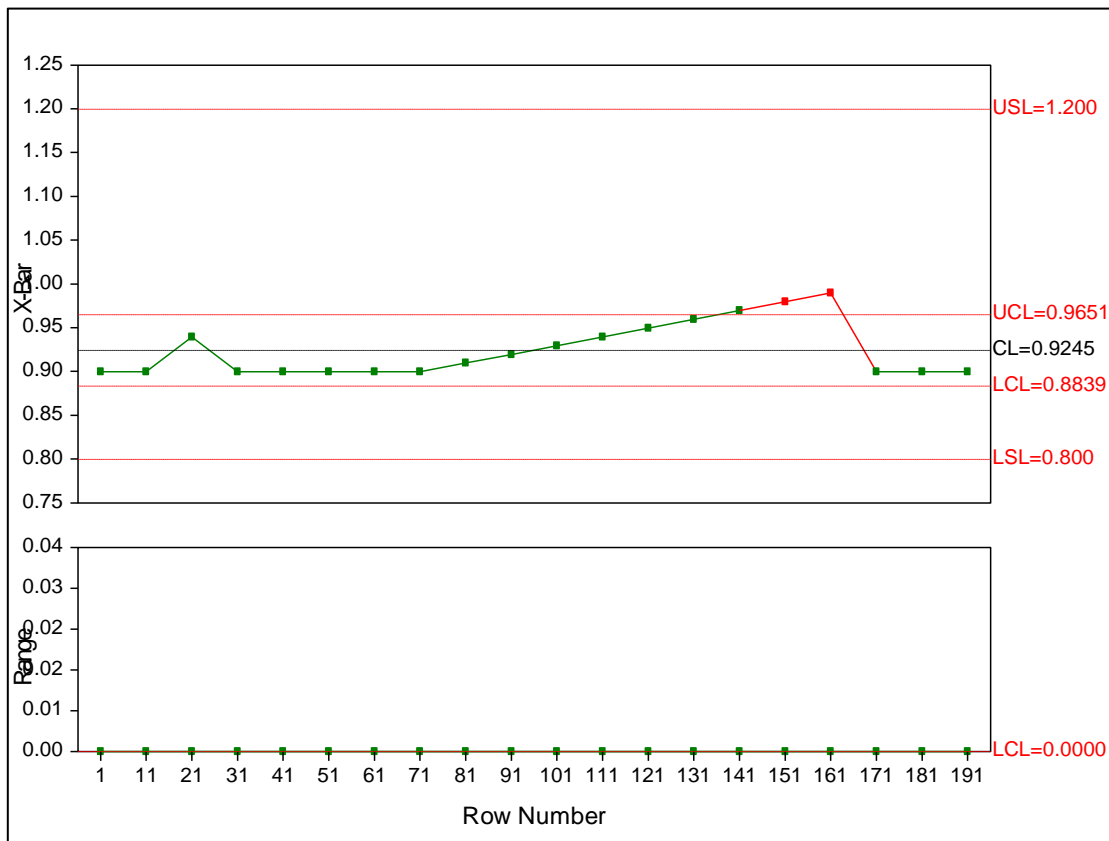


Figure 14. QIA control chart displaying 8 consecutive points rising.

**Table 1.** Limits for Figures 1 to 8 constructed using SPC for Excel and QIA.

Test	Software	Fig.	Mean	SD	USL	UCL	UWL	LWL	LCL	LSL
Normal	SPC	1	1.0039	0.1003	1.500	1.3048	1.2045	0.8032	0.7029	0.500
	QIA	2	1.0039	0.1003	1.500	1.3048	1.2045	0.8032	0.7029	0.500
1 away spec limits	SPC	3	1.0089	0.1133	1.500	1.3488	1.2355	0.7822	0.6689	0.500
	QIA	4	1.0089	0.1133	1.500	1.3488	1.2355	0.7822	0.6689	0.500
1 away 3 SD	SPC	5	1.0069	0.1055	1.500	1.3233	1.2179	0.7959	0.6904	0.500
	QIA	6	1.0069	0.1055	1.500	1.3233	1.2179	0.7959	0.6904	0.500
2 of 2 away 2 SD	SPC	7	1.0081	0.1066	1.500	1.3278	1.2212	0.7949	0.6883	0.500
	QIA	8	1.0081	0.1066	1.500	1.3278	1.2212	0.7949	0.6883	0.500

**Table 2.** Observed differences between SPC for Excel and QIA for individual control charting.

Item	SPC for Excel	Qi Analyst
<b>1</b>	For 2 of 2 consecutive points outside 2 SD away from the mean, both points are highlighted red, once the second point has been entered.	For 2 of 2 consecutive points outside 2 SD away from the mean, only the last point is highlighted red.
<b>2</b>	Points which are outside the specified limits, and within control limits are not highlighted red. User has to manually highlight points as failures in accordance with an Analytical Quality Control Procedure (AGN 1.7).	Points outside specified limits and within control limits are highlighted red.

Table 3. Summary results for randomly generated dataset in subgroups of 10

Chart type	Average	UCL	LCL
SPC for Excel Xbar chart	1.004	1.094	0.914
QIA Xbar chart	1.004	1.099	0.909
SPC for Excel R chart	0.293	0.520	0.065
QIA R chart	0.293	0.549	0.069

Table 4. Observed differences between SPC for Excel and QIA for BMMC control charting.

Item	SPC for Excel	Qi Analyst
<b>1</b>	Calculates the control limits by taking the SD of the averaged points from each run date.	The control limits are based upon the SD calculated from every individual point from the column containing all QC results.
<b>2</b>	Only calculates the average of all individual points enabled within a given subgroup. (E.g. AIQC10 runde 31/05/2017, compare QIA and SPC for Excel).	The BMMC charts average is calculated based on all the points within a subgroup regardless of the individual point being disabled.
<b>3</b>	SPC for Excel will automatically create three SD UCL and LCL limits. However, the specified limits defined in appropriate AGN technical procedures will be manually set. These will still be labelled UCL and LCL, which is a terminology difference to QIA.	Manually set upper and lower specified limits are labelled as USL and LSL respectively.
<b>4</b>	SPC for Excel will take the mean of as many points as occur within a batch (after using Pivot table to format). This will lead to fewer mean points where $n > 10$ occurs.	Limited to a maximum of 10 individual analyses. Further subgroups are created where $n > 10$ (e.g. $n$ total = 11, subgroup 1, $n = 10$ , subgroup 2, $n = 1$ ).
<b>5</b>	Highlights all the points contributing to the rule violation, i.e. SPC for Excel Random 10 of 11 sheet from Figure 13 has 9/20 up to 19/20 highlighted as red.	Only highlights red the points that violate the rules programmed within the software, i.e. QIA Random 10 of 11 sheet from Figure 14 has only points 18/20 and 19/20 as failures, as they mark the beginning of a test rule violation, which is 10 of 11 points consecutive points on one side of the mean.

### 3 Validation using stream water sample quality control data

Batches of stream water QC samples from the GSI Tellus border project were collated. Comparative Individual and BMMC Control Charts in SPC for Excel and QIA used the collated ICS 5000 system 1 QC10 chloride results and NPOC QC10 dissolved organic carbon results as displayed from Figure 17 to Figure 20. Individual QC data for ICS5000 system 1 QC10 chloride and NPOC QC10 are displayed in Appendix 3 and 4 respectively.

The limits associated with each control chart from both QIA and SPC for Excel are summarised in Table 5. It clearly shows that the comparable limits between the corresponding charts for QIA and SPC for Excel are identical. Table 6 details the highlighted test rule violations for the individuals chart and the BMMC for ICS 5000 system 1 QC10 chloride and NPOC QC10 and how it is presented for both SPC for Excel and QIA

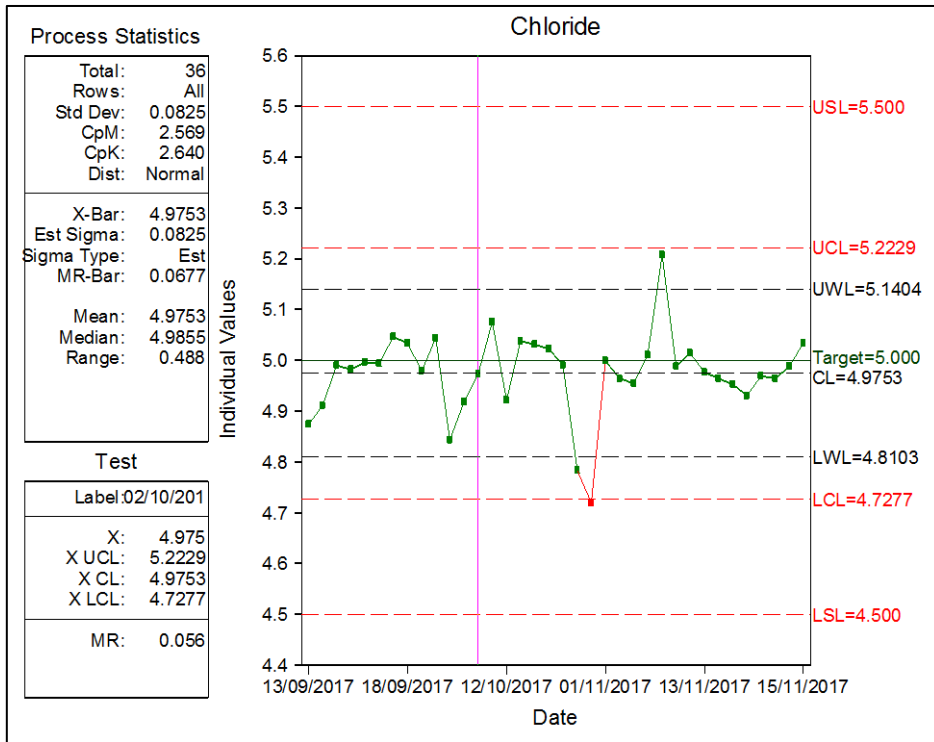


Figure 15. QIA individuals control chart for Chloride.

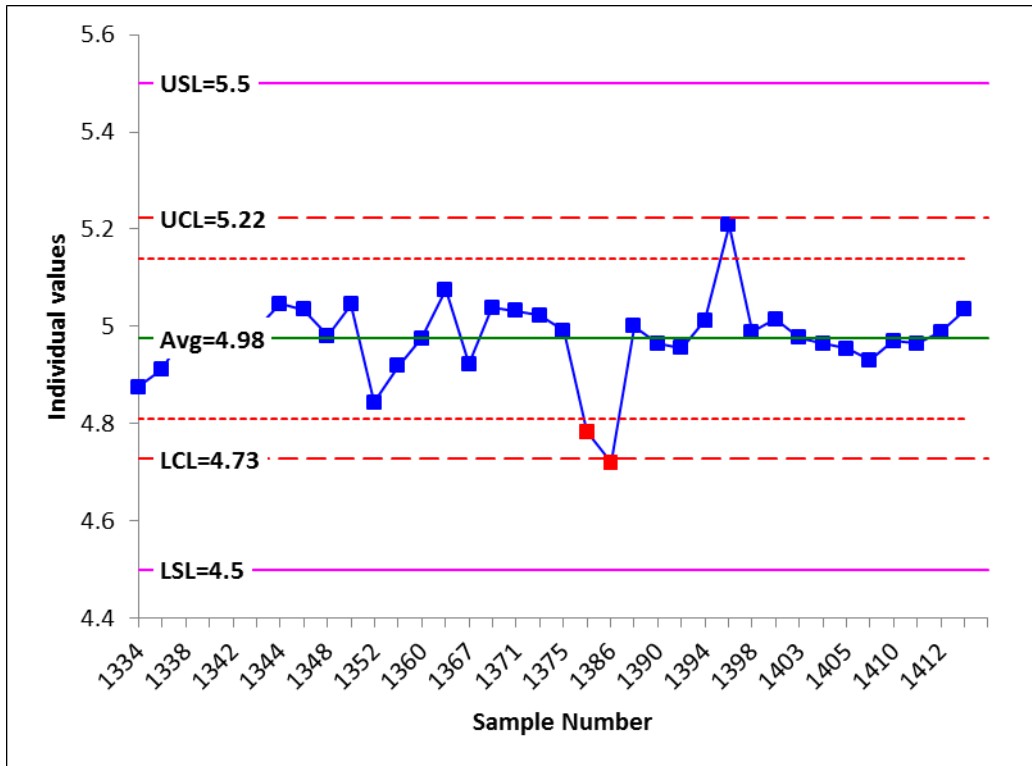


Figure 16. SPC for Excel individual control chart for Chloride.



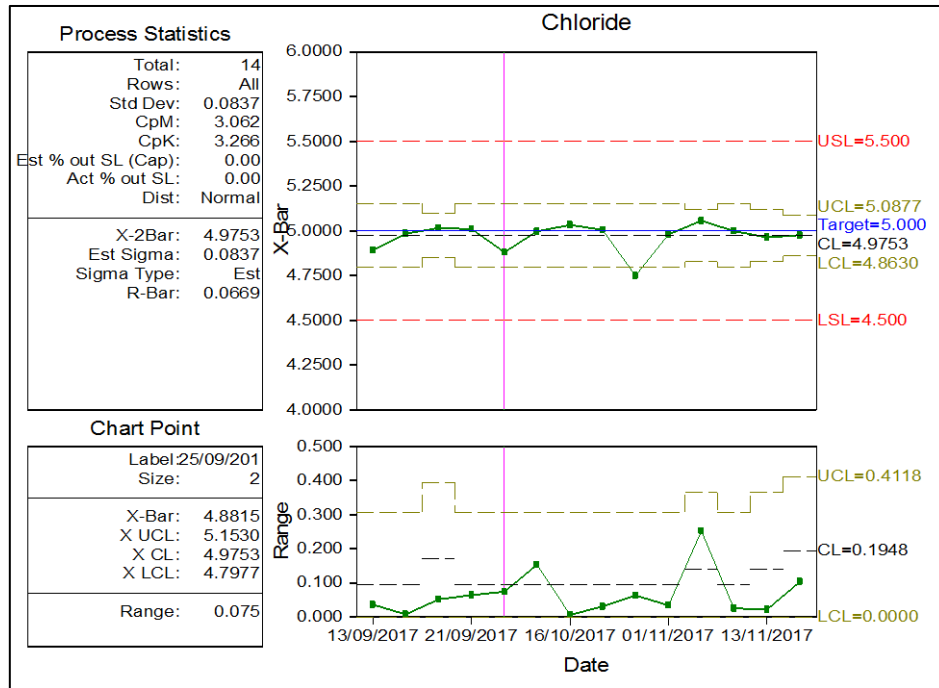


Figure 17. QIA BMMC control chart for Chloride.

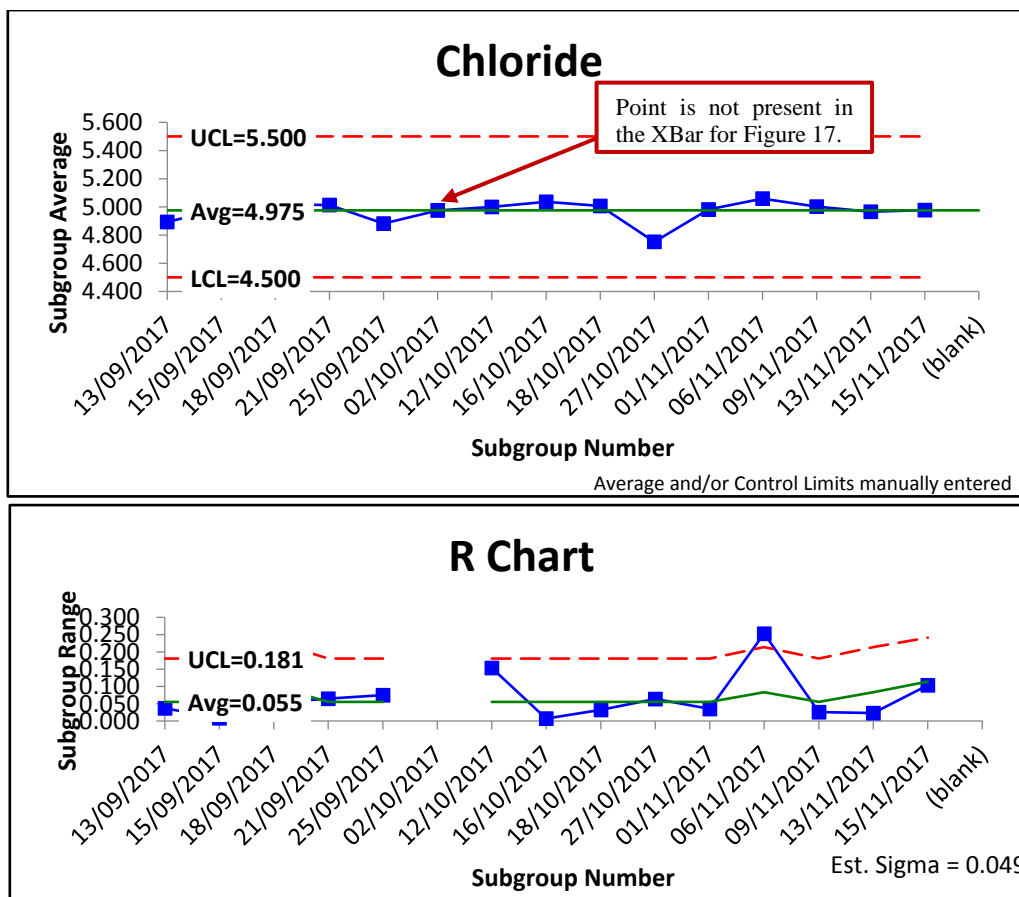


Figure 18. SPC for Excel BMMC control chart for Chloride.

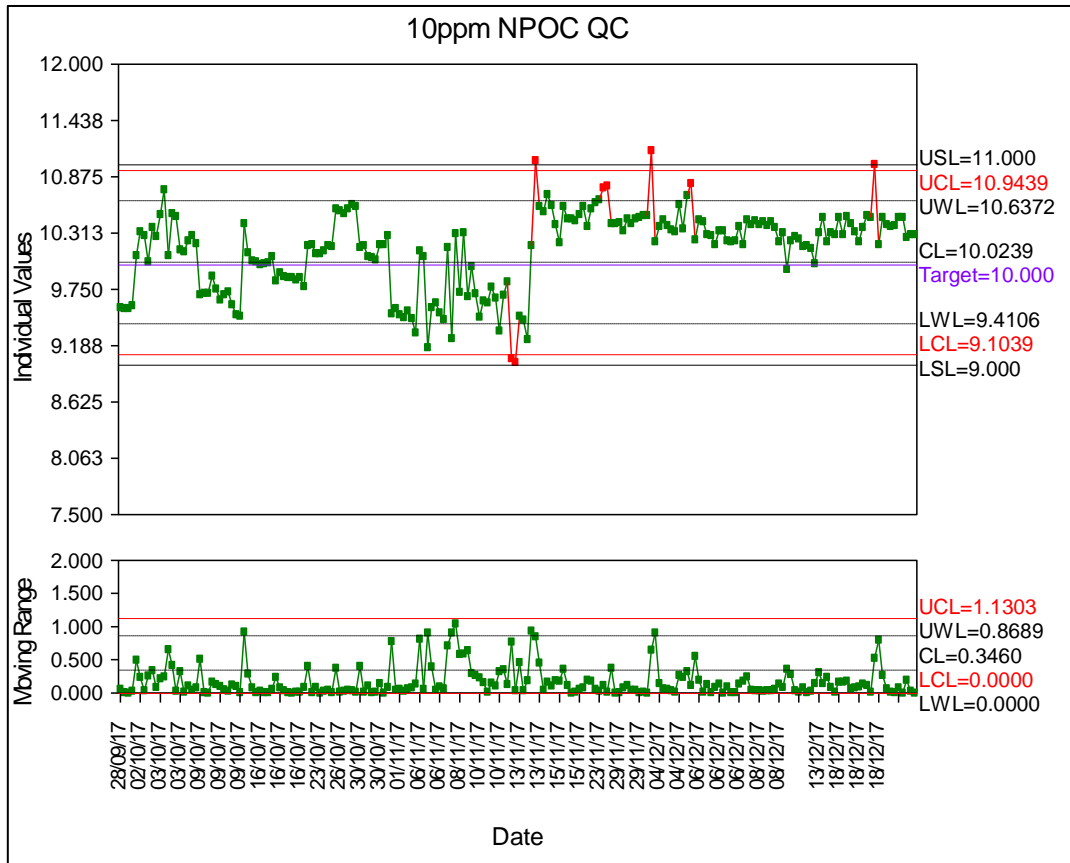


Figure 19. NPOC QC10 QIA individual control charts.

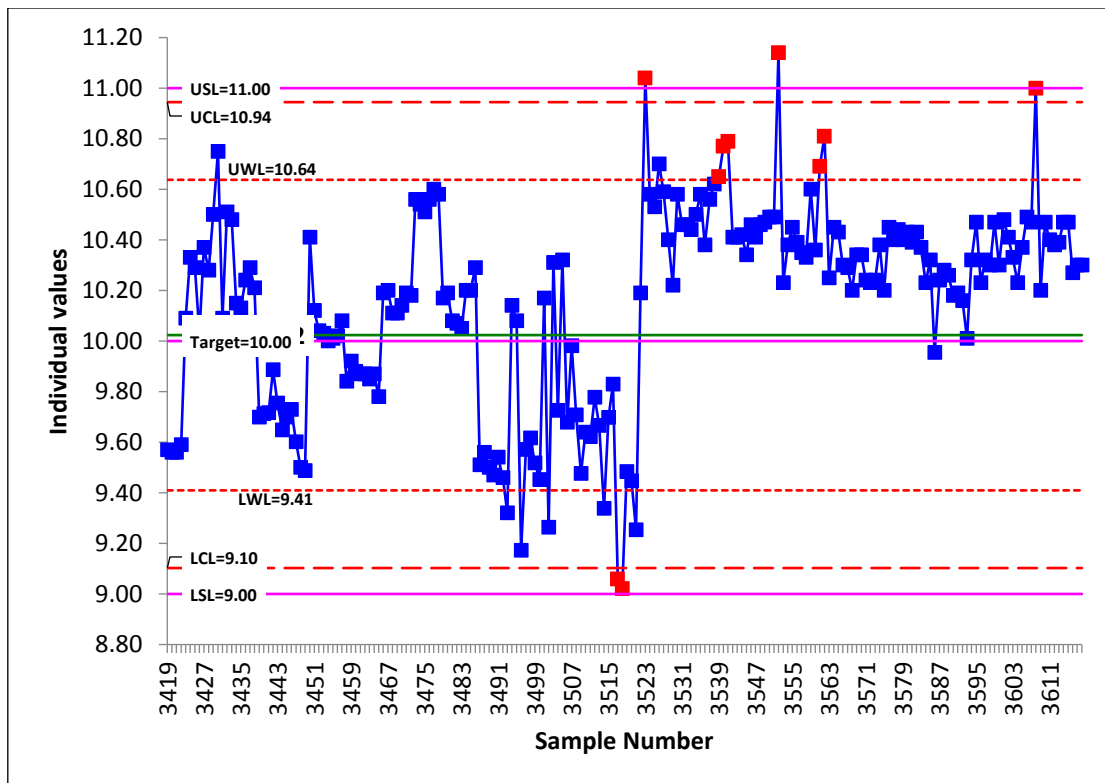


Figure 20. NPOC QC10 SPC individual control charts.

**Table 5.** Limits from Figure 15 to 18 A1 QC10 chloride Figure 19 to 20 NPOC QC10 summarised.

<b>Individual chloride chart limits</b>	<b>Fig.</b>	<b>LSL</b>	<b>LCL</b>	<b>LWL</b>	<b>CL</b>	<b>UWL</b>	<b>UCL</b>	<b>USL</b>
QIA	15	4.500	4.728	4.810	4.975	5.140	5.223	5.500
SPC for Excel	16	4.500	4.728	4.810	4.975	5.140	5.223	5.500
<b>BMMC chloride Xbar chart limits</b>	<b>Fig.</b>	<b>LSL</b>	<b>LCL</b>	<b>LWL</b>	<b>CL</b>	<b>UWL</b>	<b>UCL</b>	<b>USL</b>
QIA	17	4.500	4.863	n.a.	4.975	n.a.	5.088	5.500
SPC for Excel	18	4.500	n.a	n.a.	4.975	n.a.	n.a	5.500
<b>Individual NPOC chart limits</b>	<b>Fig.</b>	<b>LSL</b>	<b>LCL</b>	<b>LWL</b>	<b>CL</b>	<b>UWL</b>	<b>UCL</b>	<b>USL</b>
QIA	19	9.00	9.10	9.41	10.02	10.64	10.94	11.00
SPC for Excel	20	9.00	9.10	9.41	10.02	10.64	10.94	11.00

**Table 6.** Observed differences between SPC and QIA for “real” sample control charting.

<b>Item</b>	<b>SPC for Excel</b>	<b>Qi Analyst</b>
<b>1</b>	Figure 16 and Figure 20 displays a test rule violation of a 2 of 2 outside the warning limit from SPC for Excel. Both consecutive points outside the warning limits are highlighted.	Figure 15 shows how QIA only highlights the last point from the 2 of 2 outside the warning limit.
<b>2</b>	Figure 20 displays points outside the control limits which are highlighted similarly to QIA.	Figure 19 highlights points outside the control limits similarly to Figure 20.
<b>3</b>	Figure 20 points outside the specified limits are highlighted accordingly. Merely because of the points residing outside the control limits.	Figure 19 highlights specified limits as programmed in the software.
<b>4</b>	As displayed in Figure 18 if only a single result is recorded on a given calibration run, the point is still plotted on the XBar chart and is left blank in the R chart as shown in Figure 18.	From the BMMC chart, if only a single result is recorded on a given calibration run, the point is not plotted on the Xbar chart and is not present in the R chart as shown in Figure 17 and noted in Figure 18.
<b>5</b>	The limits established for Figure 18 only displays the UCL and LCL which are equivalent to USL and LSL in QIA respectively.	QIA displays both UCL, LCL, USL, and LSL as shown in Figure 17.

## 4 Summary of terminology used in QIA (version 3.5, 1998) and SPC for Excel (version 5, 2017)

### 4.1 INDIVIDUALS CHARTS

USL and LSL	Mean $\pm$ expanded uncertainty.
UCL and LCL	Defined as the intervals three SD above and below the mean respectively
UWL and LWL	Defined as the intervals two SD above and below the mean respectively
Average	Average of all the accepted QC datapoints encompassing the chart
CL	The target value around which the SLs have been set

### 4.2 BMMC

There is only one terminology difference between QIA and SPC for Excel which occurs in the BMMC. In SPC for Excel, UCL is the direct equivalent to USL in QIA and the same is true for LCL and LSL.

USL and LSL (Used in QIA)	Mean $\pm$ expanded uncertainty.
UCL and LCL (Equivalent to USL and LSL in QIA)	Automated setup is defined as the intervals three SD above and below the mean respectively. Manual setup in SPC for Excel defines these lines under an authorised persons discretion.
UWL and LWL	Defined as the intervals two SD above and below the mean respectively
Average	Average of all the accepted QC datapoints encompassing the chart
CL	The target value around which the SLs have been set
Moving range	The difference between the current observed QC result and the observed QC result immediately prior.

## 5 Conclusions

SPC for Excel (version 5, 2017) has been successfully validated against the existing legacy QC software (version 3.5, 1998), demonstrating conformance to UKAS accreditation requirements.

There are minor operational differences which are detailed above in Table 2 and Table 4.

The individual control charts produced in QIA are reproducible in SPC for Excel in relation to the data plotting and limit calculation. Visualisation of rule violations is different in that 2 of 2 consecutive points outside the warning limits are highlight for SPC for Excel, however QIA only highlights the last of the two points as stated in Table 2. In the event that the control limits extend beyond the specified limits, manual intervention is required in SPC for Excel to disable datapoints which fall between the specified limits and the control limits. Previously in QIA this was an automatic test rule violation (see Table 2).

The BMMC charting in SPC is wholly consistent with the existing QIA software, unless there are more than 10 datapoints per batch (Table 4 item 4). The summary statistical values presented on the graph, e.g. the average, are then calculated differently in the software with a minor difference with the standard deviations rising (Table 4 item 1). This will increase the efficiency of the BMMC test.

The BMMC reference lines are not used in decision making and are provided for visual purposes only. Difference in visualisation of these data are also highlighted in

Table 4.

To conclude, using the SPC for Excel program is suitable for UKAS accredited standards as specified in an Analytical Quality Control procedure (AGN 1.7).

## 6 References

AGN 1.7. Analytical Quality Control. Inorganic Geochemistry Team UKAS Operating Procedure (version 10.0; 2012).

SPC for Excel (2007). Instruction Manual for SPC for MS Excel V3.0. *Business Process Improvement*.

SPSS QI Analyst Software 1998. Version 3.5.2.

# Appendix 1 Synthetic datasets utilised for constructing individual control charts

Synthetic randomly generated dataset for individual control charting.

Number sequence	Random	1 away spec limits	1 away 3 sigma	2 of 2 away 2 sigma
1	1.0315	1.5315	1.3315	1.2515
2	1.0778	1.0778	1.0778	1.2778
3	1.0420	1.0420	1.0420	1.0420
4	1.0762	1.0762	1.0762	1.0762
5	1.0239	1.0239	1.0239	1.0239
6	0.9834	0.9834	0.9834	0.9834
7	0.9476	0.9476	0.9476	0.9476
8	1.0800	1.0800	1.0800	1.0800
9	1.0529	1.0529	1.0529	1.0529
10	0.9668	0.9668	0.9668	0.9668
11	0.9067	0.9067	0.9067	0.9067
12	0.7962	0.7962	0.7962	0.7962
13	1.0259	1.0259	1.0259	1.0259
14	1.0618	1.0618	1.0618	1.0618
15	1.1257	1.1257	1.1257	1.1257
16	0.9523	0.9523	0.9523	0.9523
17	1.2623	1.2623	1.2623	1.2623
18	0.9980	0.9980	0.9980	0.9980
19	0.9556	0.9556	0.9556	0.9556
20	1.0426	1.0426	1.0426	1.0426
21	1.2574	1.2574	1.2574	1.2574
22	1.1183	1.1183	1.1183	1.1183
23	1.1107	1.1107	1.1107	1.1107
24	1.0763	1.0763	1.0763	1.0763
25	1.0062	1.0062	1.0062	1.0062
26	1.0085	1.0085	1.0085	1.0085
27	1.0794	1.0794	1.0794	1.0794
28	1.0122	1.0122	1.0122	1.0122
29	0.9430	0.9430	0.9430	0.9430
30	1.1729	1.1729	1.1729	1.1729
31	1.1261	1.1261	1.1261	1.1261
32	1.0215	1.0215	1.0215	1.0215
33	1.0563	1.0563	1.0563	1.0563
34	1.1583	1.1583	1.1583	1.1583
35	1.0447	1.0447	1.0447	1.0447
36	0.9504	0.9504	0.9504	0.9504
37	1.0522	1.0522	1.0522	1.0522
38	0.9856	0.9856	0.9856	0.9856

Number sequence	Random	1 away spec limits	1 away 3 sigma	2 of 2 away 2 sigma
39	1.1452	1.1452	1.1452	1.1452
40	1.0943	1.0943	1.0943	1.0943
41	0.8534	0.8534	0.8534	0.8534
42	0.9691	0.9691	0.9691	0.9691
43	0.9306	0.9306	0.9306	0.9306
44	1.1168	1.1168	1.1168	1.1168
45	0.9924	0.9924	0.9924	0.9924
46	1.0056	1.0056	1.0056	1.0056
47	1.0039	1.0039	1.0039	1.0039
48	0.9317	0.9317	0.9317	0.9317
49	0.8694	0.8694	0.8694	0.8694
50	1.0604	1.0604	1.0604	1.0604
51	0.9422	0.9422	0.9422	0.9422
52	0.9687	0.9687	0.9687	0.9687
53	1.1086	1.1086	1.1086	1.1086
54	1.1211	1.1211	1.1211	1.1211
55	0.9726	0.9726	0.9726	0.9726
56	0.9566	0.9566	0.9566	0.9566
57	0.9705	0.9705	0.9705	0.9705
58	0.9762	0.9762	0.9762	0.9762
59	0.8121	0.8121	0.8121	0.8121
60	0.9857	0.9857	0.9857	0.9857
61	1.0247	1.0247	1.0247	1.0247
62	1.0786	1.0786	1.0786	1.0786
63	1.0110	1.0110	1.0110	1.0110
64	0.9455	0.9455	0.9455	0.9455
65	0.9136	0.9136	0.9136	0.9136
66	0.9878	0.9878	0.9878	0.9878
67	1.0826	1.0826	1.0826	1.0826
68	1.0166	1.0166	1.0166	1.0166
69	1.1144	1.1144	1.1144	1.1144
70	1.1636	1.1636	1.1636	1.1636
71	0.8858	0.8858	0.8858	0.8858
72	0.8809	0.8809	0.8809	0.8809
73	1.1388	1.1388	1.1388	1.1388
74	0.8494	0.8494	0.8494	0.8494
75	0.8397	0.8397	0.8397	0.8397
76	1.0276	1.0276	1.0276	1.0276
77	0.8761	0.8761	0.8761	0.8761
78	1.0222	1.0222	1.0222	1.0222
79	0.9926	0.9926	0.9926	0.9926
80	0.8613	0.8613	0.8613	0.8613
81	0.9850	0.9850	0.9850	0.9850
82	1.0207	1.0207	1.0207	1.0207
83	0.9569	0.9569	0.9569	0.9569



Number sequence	Random	1 away spec limits	1 away 3 sigma	2 of 2 away 2 sigma
84	1.1673	1.1673	1.1673	1.1673
85	0.7973	0.7973	0.7973	0.7973
86	0.9123	0.9123	0.9123	0.9123
87	0.7125	0.7125	0.7125	0.7125
88	1.0094	1.0094	1.0094	1.0094
89	1.1283	1.1283	1.1283	1.1283
90	0.9613	0.9613	0.9613	0.9613
91	0.8645	0.8645	0.8645	0.8645
92	1.0429	1.0429	1.0429	1.0429
93	1.0335	1.0335	1.0335	1.0335
94	1.0682	1.0682	1.0682	1.0682
95	0.8490	0.8490	0.8490	0.8490
96	0.9514	0.9514	0.9514	0.9514
97	1.0147	1.0147	1.0147	1.0147
98	1.0809	1.0809	1.0809	1.0809
99	0.8572	0.8572	0.8572	0.8572
100	0.8838	0.8838	0.8838	0.8838

## Appendix 2 Synthetic datasets utilised for constructing BMCC control charts

Randomly generated dataset in subgroups of 10 for BMCC.

Average of Random	1	2	3	4	5	6	7	8	9	10
A	1.031	1.078	1.042	1.076	1.024	0.983	0.948	1.080	1.053	0.967
B	0.907	0.796	1.026	1.062	1.126	0.952	1.262	0.998	0.956	1.043
C	1.257	1.118	1.111	1.076	1.006	1.008	1.079	1.012	0.943	1.173
D	1.126	1.021	1.056	1.158	1.045	0.950	1.052	0.986	1.145	1.094
E	0.853	0.969	0.931	1.117	0.992	1.006	1.004	0.932	0.869	1.060
F	0.942	0.969	1.109	1.121	0.973	0.957	0.970	0.976	0.812	0.986
G	1.025	1.079	1.011	0.945	0.914	0.988	1.083	1.017	1.114	1.164
H	0.886	0.881	1.139	0.849	0.840	1.028	0.876	1.022	0.993	0.861
I	0.985	1.021	0.957	1.167	0.797	0.912	0.712	1.009	1.128	0.961
J	0.864	1.043	1.034	1.068	0.849	0.951	1.015	1.081	0.857	0.884

Generated dataset simulating 10 of 11 outside the mean test violation.

Average of Result [10 of 11]	QC1	QC2	QC3	QC4	QC5
01/11/2017	1.00	1.10	0.90	1.00	1.00
02/11/2017	1.00	1.10	0.90	1.00	1.00
03/11/2017	1.00	1.10	0.90	1.00	1.00
04/11/2017	1.00	1.10	0.90	1.00	1.00
05/11/2017	1.00	1.10	0.90	1.00	1.00
06/11/2017	1.00	1.10	0.90	1.00	1.00
07/11/2017	1.00	1.10	0.90	1.00	1.00
08/11/2017	1.00	1.10	0.90	1.00	1.00
09/11/2017	1.40	1.40	1.40	1.40	1.40
10/11/2017	1.40	1.40	1.40	1.40	1.40
11/11/2017	1.40	1.40	1.40	1.40	1.40
12/11/2017	1.40	1.40	1.40	1.40	1.40
13/11/2017	1.40	1.40	1.40	1.40	1.40
14/11/2017	1.40	1.40	1.40	1.40	1.40
15/11/2017	1.40	1.40	1.40	1.40	1.40
16/11/2017	1.40	1.40	1.40	1.40	1.40
17/11/2017	1.40	1.40	1.40	1.40	1.40
18/11/2017	1.40	1.40	1.40	1.40	1.40
19/11/2017	1.40	1.40	1.40	1.40	1.40
20/11/2017	1.00	1.10	0.90	1.00	1.00

Generated dataset simulating 8 consecutive points rising test violation.

Average of Result [8]	QC1	QC2	QC3	QC4	QC5
01/11/2017	0.90	0.90	0.90	0.90	0.90
02/11/2017	0.90	0.90	0.90	0.90	0.90
03/11/2017	0.94	0.94	0.94	0.94	0.94
04/11/2017	0.90	0.90	0.90	0.90	0.90
05/11/2017	0.90	0.90	0.90	0.90	0.90
06/11/2017	0.90	0.90	0.90	0.90	0.90
07/11/2017	0.90	0.90	0.90	0.90	0.90
08/11/2017	0.90	0.90	0.90	0.90	0.90
09/11/2017	0.91	0.91	0.91	0.91	0.91
10/11/2017	0.92	0.92	0.92	0.92	0.92
11/11/2017	0.93	0.93	0.93	0.93	0.93
12/11/2017	0.94	0.94	0.94	0.94	0.94
13/11/2017	0.95	0.95	0.95	0.95	0.95
14/11/2017	0.96	0.96	0.96	0.96	0.96
15/11/2017	0.97	0.97	0.97	0.97	0.97
16/11/2017	0.98	0.98	0.98	0.98	0.98
17/11/2017	0.99	0.99	0.99	0.99	0.99
18/11/2017	0.90	0.90	0.90	0.90	0.90
19/11/2017	0.90	0.90	0.90	0.90	0.90
20/11/2017	0.90	0.90	0.90	0.90	0.90

## Appendix 3 ICS 5000 System 1 QC10 chloride results

QC dataset for individual results utilised for individual control charting

Date	Name	Chloride
13/09/2017	QC12/10	4.875
13/09/2017	QC15/10	4.912
15/09/2017	QC09/10	4.991
15/09/2017	QC12/10	4.983
18/09/2017	QC09/10	4.997
18/09/2017	QC12/10	4.994
18/09/2017	QC15/10	5.047
18/09/2017	QC18/10	5.034
21/09/2017	QC09/10	4.98
21/09/2017	QC12/10	5.045
25/09/2017	QC09/10	4.844
25/09/2017	QC12/10	4.919
02/10/2017	QC12/10	4.975
12/10/2017	QC09/10	5.076
12/10/2017	QC12/10	4.922
16/10/2017	QC09/10	5.039
16/10/2017	QC12/10	5.032
18/10/2017	QC09/10	5.023
18/10/2017	QC12/10	4.991
27/10/2017	QC09/10	4.784
27/10/2017	QC12/10	4.720
01/11/2017	QC09/10	5.000
01/11/2017	QC12/10	4.965
06/11/2017	QC09/10	4.955
06/11/2017	QC12/10	5.012
06/11/2017	QC15/10	5.208
09/11/2017	QC09/10	4.989
09/11/2017	QC12/10	5.015
13/11/2017	QC12/10	4.977
13/11/2017	QC15/10	4.965
13/11/2017	QC18/10	4.954
15/11/2017	QC12/10	4.931
15/11/2017	QC15/10	4.970
15/11/2017	QC18/10	4.965
15/11/2017	QC21/10	4.988
15/11/2017	QC24/10	5.035

## QC dataset of individual results reformatted for BMMC charting

Average of Chloride							
	QC09/10	QC12/10	QC15/10	QC18/10	QC21/10	QC24/10	(blank)
13/09/2017		4.875	4.912				
15/09/2017	4.991	4.983					
18/09/2017	4.997	4.994	5.047	5.034			
21/09/2017	4.980	5.045					
25/09/2017	4.844	4.919					
02/10/2017		4.975					
12/10/2017	5.076	4.922					
16/10/2017	5.039	5.032					
18/10/2017	5.023	4.991					
27/10/2017	4.784	4.720					
01/11/2017	5.000	4.965					
06/11/2017	4.955	5.012	5.208				
09/11/2017	4.989	5.015					
13/11/2017		4.977	4.965	4.954			
15/11/2017		4.931	4.970	4.965	4.988	5.035	
(blank)							

## Appendix 4 NPOC QC10 dissolved organic carbon results

NPOC QC10 dataset of individual results displayed for individual control charting\*

Number	Date	QC10	Number	Date	QC10	Number	Date	QC10
3520	13/11/2017	9.45	3557	04/12/2017	10.35	3594	13/12/2017	10.32
3521	13/11/2017	9.25	3558	04/12/2017	10.33	3595	13/12/2017	10.47
3522	13/11/2017	10.19	3559	04/12/2017	10.60	3596	13/12/2017	10.23
3523	13/11/2017	11.04	3560	04/12/2017	10.36	3597	13/12/2017	10.32
3524	13/11/2017	10.58	3561	04/12/2017	10.69	3598	13/12/2017	10.30
3525	15/11/2017	10.53	3562	04/12/2017	10.81	3599	18/12/2017	10.47
3526	15/11/2017	10.70	3563	04/12/2017	10.25	3600	18/12/2017	10.30
3527	15/11/2017	10.59	3564	06/12/2017	10.45	3601	18/12/2017	10.48
3528	15/11/2017	10.40	3565	06/12/2017	10.43	3602	18/12/2017	10.41
3529	15/11/2017	10.22	3566	06/12/2017	10.30	3603	18/12/2017	10.33
3530	15/11/2017	10.58	3567	06/12/2017	10.29	3604	18/12/2017	10.23
3531	15/11/2017	10.46	3568	06/12/2017	10.20	3605	18/12/2017	10.37
3532	15/11/2017	10.46	3569	06/12/2017	10.34	3606	18/12/2017	10.49
3533	15/11/2017	10.44	3570	06/12/2017	10.34	3607	18/12/2017	10.47
3534	15/11/2017	10.50	3571	06/12/2017	10.24	3608	18/12/2017	11.00
3535	15/11/2017	10.58	3572	06/12/2017	10.23	3609	18/12/2017	10.20
3536	15/11/2017	10.38	3573	06/12/2017	10.24	3610	18/12/2017	10.47
3537	23/11/2017	10.56	3574	06/12/2017	10.38	3611	18/12/2017	10.40
3538	23/11/2017	10.62	3575	06/12/2017	10.20	3612	18/12/2017	10.38
3539	23/11/2017	10.65	3576	08/12/2017	10.45	3613	18/12/2017	10.39
3540	23/11/2017	10.77	3577	08/12/2017	10.40	3614	18/12/2017	10.47
3541	23/11/2017	10.79	3578	08/12/2017	10.44	3615	21/12/2017	10.47
3542	29/11/2017	10.41	3579	08/12/2017	10.40	3616	21/12/2017	10.27
3543	29/11/2017	10.41	3580	08/12/2017	10.43	3617	21/12/2017	10.30
3544	29/11/2017	10.42	3581	08/12/2017	10.39	3618	21/12/2017	10.30
3545	29/11/2017	10.34	3582	08/12/2017	10.43			
3546	29/11/2017	10.46	3583	08/12/2017	10.37			
3547	29/11/2017	10.41	3584	08/12/2017	10.23			
3548	29/11/2017	10.46	3585	08/12/2017	10.32			
3549	29/11/2017	10.47	3586	08/12/2017	9.95			
3550	29/11/2017	10.49	3587	08/12/2017	10.24			
3551	29/11/2017	10.49	3588	08/12/2017	10.28			
3552	29/11/2017	11.14	3589	08/12/2017	10.26			
3553	04/12/2017	10.23	3590	08/12/2017	10.18			
3554	04/12/2017	10.38	3591	13/12/2017	10.19			
3555	04/12/2017	10.45	3592	13/12/2017	10.16			
3556	04/12/2017	10.39	3593	13/12/2017	10.01			

\*The dataset shown on the table only displays what is shown on the control chart in Figure 19 and Figure 20. However, the setup of the control and warning limits take into account results spanning 2007 to 2017.

## Appendix 5 Instruction Manual for Constructing Control Charts in SPC for Excel



Inorganic Geochemistry Department.  
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**Aim:** To provide instruction to construct control charts that perform QC checks within the standards governed by a Analytical Quality Control procedure (AGN 1.7).

### **Summary:**

SPC for Excel version 5, 2017 (SPC for Excel) replaces QI Analyst version 3.5, 1997 (QIA) to monitor the performance of QC during the analysis of unknown samples in accordance with AGN 1.7 procedures. A companion document (“Validation of SPC for Excel”) documents the validation for reproducibility between the two software systems, and more importantly the compliance of SPC within an Analytical Quality Control procedure (AGN 1.7). This document provides instructions for users to update existing QC charts with new data, how to exclude any unfit data points, and maintain a log of these. Additionally, instructions are included for creating new QC charts.

This document details plotting SPC for Excel control charts for:

- Individuals
- Batch mean measurement chart (BMMC)

The instructions include the use of Excel pivot tables to structure data for plotting BMMC charts and the re-formatting of legacy data from QIA.

These instructions are suitable for any methods used in Inorganic Geochemistry: SPC for Excel has a capacity for 7 analytes, equivalent to 14 chart sheets, 2 file sheets and 1 notes section sheet simultaneously in one file. Thus, is suitable for transitioning ion chromatography QC data from QIA to SPC.

## Accessing SPC for Excel

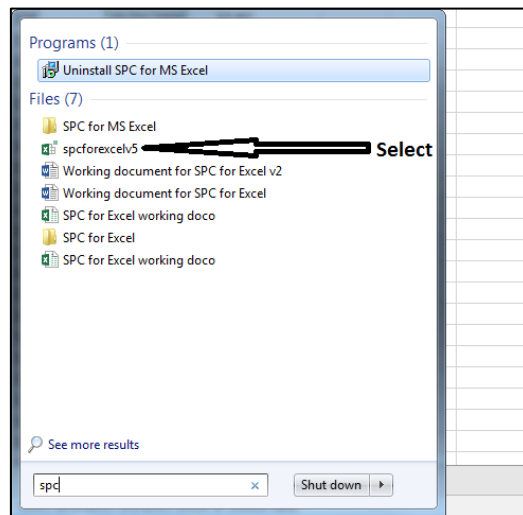
### Licensed computer to remote access

If working from a computer without license to the SPC for Excel add-in package, one can remote access to that PC.

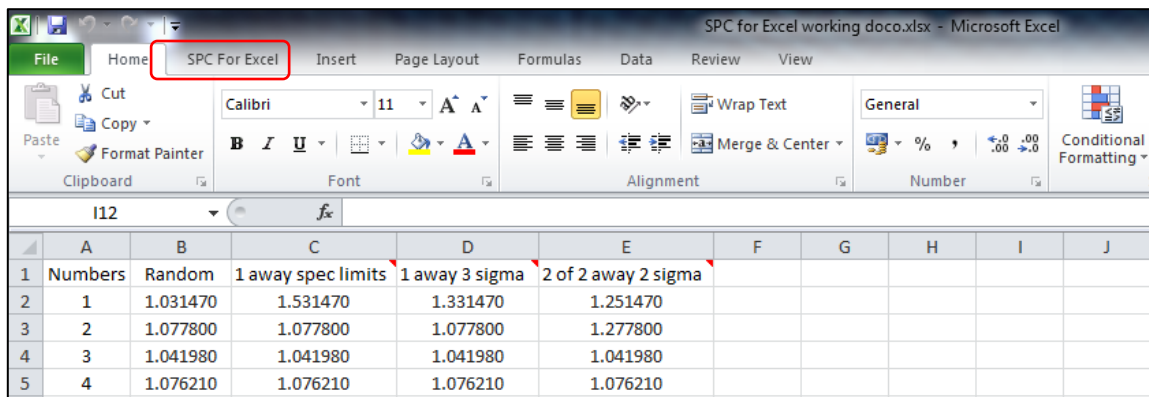
From windows select 'Remote Desktop Connection' and copy and paste the licensed computer ID stated above.

### Initial setup of SPC for Excel

The aim of this section is to instruct the user how to create and utilise Levey Jennings chart from the SPC for Excel add-in. First of all, to access the correct excel document, go to programs and search for 'spc'. Select the option called 'spcforexcelv5' as shown in Figure . This will embed the program as an add-in tab for subsequently opened excel files as shown in Figure 2 .



**Figure 1.** File to select in order to begin Levey-Jennings chart construction.



**Figure 2 .** Screen capture of accessible add in SPC for excel as indicated by red outline.

\*For instruction purposes, randomly generated values from prior document are used to demonstrate control chart construction.

Bear in mind that although the SPC for Excel add-in will only be available from a licensed computer for updating of charts, all data and constructed charts will be observable from any network connected computer.

## Constructing a new Levey-Jennings chart (Individuals control chart)

Selecting the SPC for Excel tab opens various options, as shown in Figure . The options highlighted are used to carry out functions to construct both control charts needed for QC checks specified in AGN 1.7.

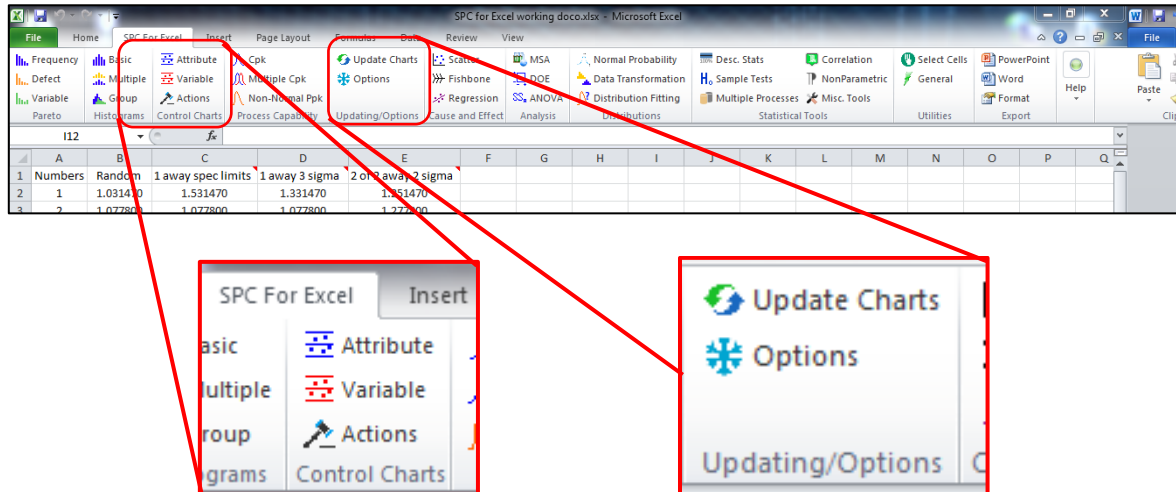


Figure 3. SPC for Excel options of interest.

### Constructing a Levey-Jennings chart:

1. As shown in Figure from the control charts menu, select variable. This will pop up 'Variable Control Charts' as shown in Figure 4

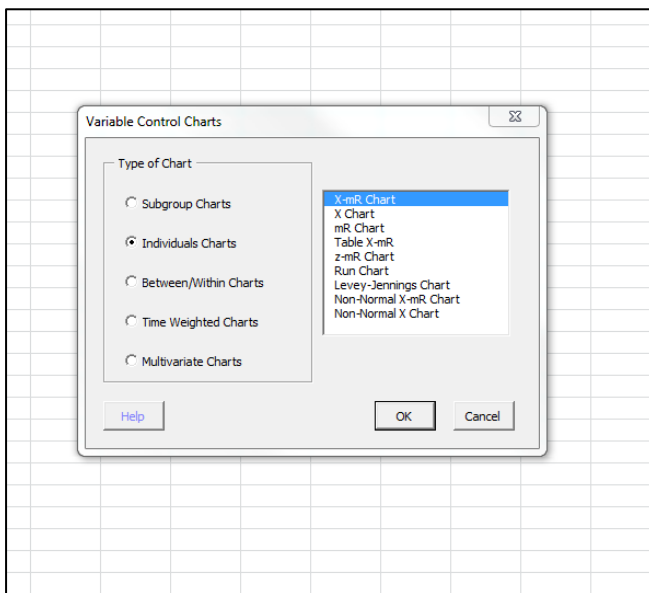


Figure 4. Various control chart options.

2. Select Individual charts, followed by the Levey-Jennings chart.
3. An additional pop up will appear as shown in Figure 5. Options will be available to the user, namely: Ranges, Chart input and Options. Set these parameters as explained below.

**Ranges:** Sample identifiers (Labels given to every data. This would normally be the unique sequential number allocated for a result or its date).

**Chart input:** Select sample identifiers & data as 'In one column'. Have 'Yes' selected for automatic updating of limits.

**Options:** Various parameters may be adjusted from the options menu. Important sections to set are found in 'out of control test' and 'control limit options' as shown in

Figure and Figure should one wish to amend chart format or display, select 'titles and formats'. The 'chart location' gives the option of selecting where the chart will be constructed i.e. new workbook or new sheet.

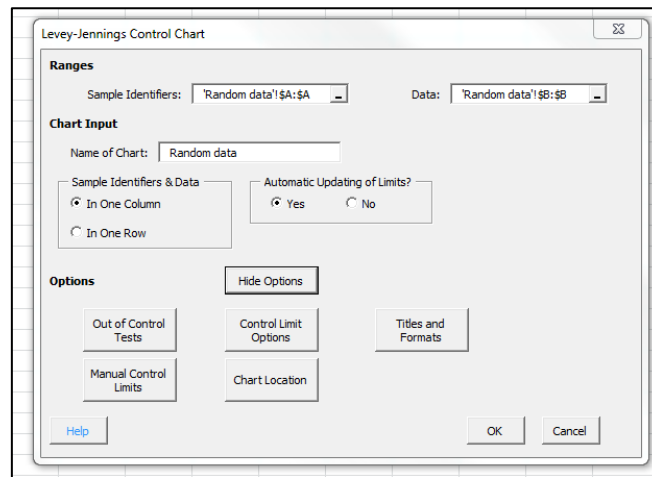


Figure 5. Levey-Jennings chart options.

4. To determine what is considered in or out of control for the control charts, the rules need to be set up by selecting the 'out of control tests' option, as shown in Figure 5
5. The popup shown in Figure will then appear. In order to test using control chart rules as outlined by an Analytical Quality Control procedure (AGN 1.7), the first and third boxes shown in Figure will need to be selected and the K value for the third section valued at 2.

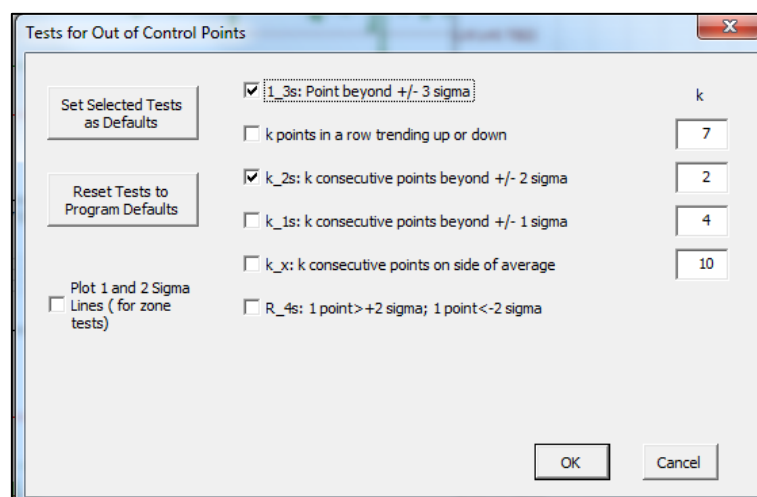


Figure 6. Test rule violation users could set to determine pass or fails on control chart.

6. By selecting the 'out of control limit' options shown in Figure 5, a pop up as displayed in Figure will appear. In order to test against control chart rules as outlined by AGN 1.7 the following parameters will need to be set:
  - Base control limits on +/- set to 3 sigma
  - Additional Lines for Levey-Jennings chart: First set to 2 sigma
  - Enter specification limits as the specified uncertainty limits. Specification limits are calculated based upon the expanded uncertainty (rounded up) documented and measured from the validation procedure protocol. The expanded uncertainty is the measured uncertainty multiplied by a factor of two. The measured uncertainty is calculated as the square root of the sum of squares of both the measured bias (%) and precision (%) for a particular analyte at a specific concentration.

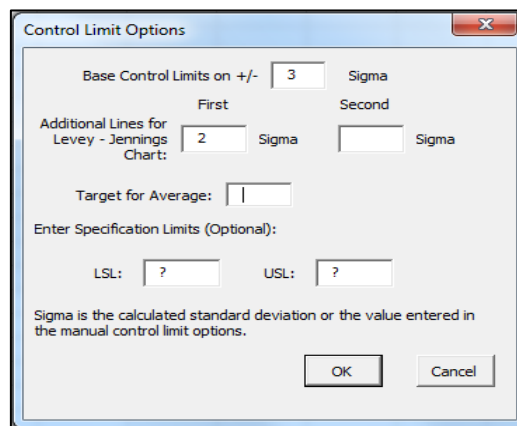


Figure 7. Where borders are set for the control charts to indicate control limits.

7. Once parameters are set for the Levey-Jennings control chart, the chart is produced as shown in Figure . In summary, USL and LSL (arbitrary specified limits) are shown as 1.5 and 0.5 respectively, the control limits (3 SD away from the mean on either side) and working limits (2 SD away from the mean on either side) are calculated and displayed as red dashed lines based on the standard deviation of the total randomly generated dataset.

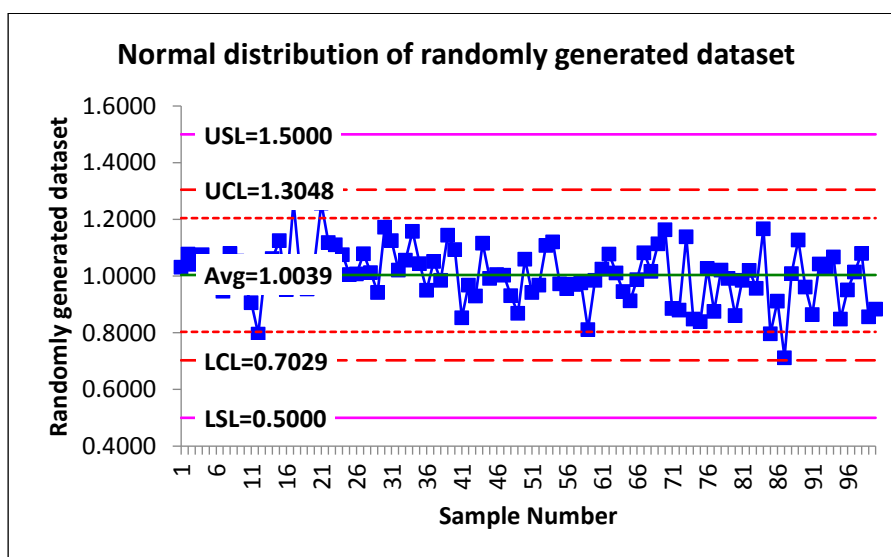
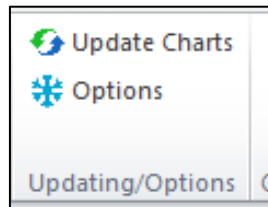


Figure 8. Control chart produced as instructed by constructing a basic Levey-Jennings chart.

## Updating existing Levey-Jennings chart (Individual control charts)

As charts are already constructed for most of the instruments QC checks for the U030 laboratories, the crucial information for a regular user will be the task of adding new QC results and updating the charts from these worksheets.

As the chart is constantly updated as new QC results are entered, the following steps will need to be followed in order to keep the charts up to date:



**Figure 9.** Updating options in SPC add on.

1. The updating options as shown in Figure (also shown in Figure 9 above) will be utilised to achieve this.
2. From a raw data sheet as exemplified in Figure , where all QC data is stored, add data points to empty cells as directed.

Number sequence ▾	Random ▾	Notes ▾
82	1.0207	
83	0.9569	
84	1.1673	
85	0.7973	
86	0.9123	
87	0.7125	
88	1.0094	
89	1.1283	
90	0.9613	
91	0.8645	
92	1.0429	
93	1.0335	
94	1.0682	
95	0.8490	
96	0.9514	
97	1.0147	
98	1.0809	
99	0.8572	
100	0.8838	
UNIQUE ID OR SEQUENTIAL NUMBERING HERE	NEW QC RESULTS HERE	

**Figure 10.** Entering new QC data.

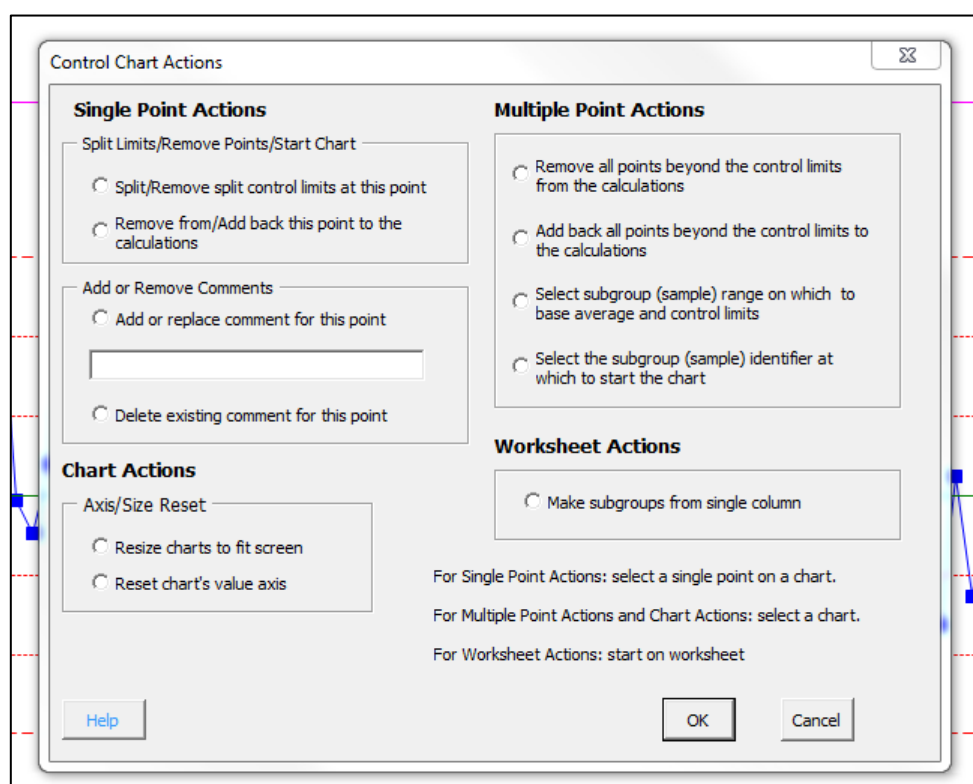
3. When new datapoints are added to a sheet connected to a control chart, select 'update charts' from updating options as shown in Figure .
4. This will prompt a pop up asking whether to update all available charts, or only specifically selected charts. For convenience select update all.
5. Afterwards, the control charts associated with the columns where new data has been inserted will now have new points plotted at the end.
6. As a consequence, the UCL, LCL, 2 and 3 sigma border will also expand or contract as influenced by the newly added datapoints.

## Actions for existing Levey-Jennings chart (Individual control charts)

In the event that certain changes are required for a given chart, open the sheet for the chart in question and proceed to select the 'actions' from control chart (Refer to Figure ). Figure below shows the options available once the 'action' option is selected.

Some events that could warrant using the 'actions' option include:

- Failures requiring the addition of comments and/or removal of a given datapoint
- Changing the chart format to observe datapoints which are most recent
- Step changes required based on QC reviews (Rare)



**Figure 11.** Pop up appears once 'Actions' from control charts options is selected.



## Control chart actions options

A point can be individually selected from a given chart, which will prompt several actions to be conducted from the Control Chart Actions menu. The options shown in Figure 11 are further detailed below.

**Single point actions:** The option to 'split/remove split control limits at this point' will only be used in the event of a significant systematic change in the overall performance of the QC results over an extended period of time, evidenced with a significant number of calibration runs with QC results. In the event that the experienced analyst or lab manager does deem it necessary to 'split the control limits', the authorised approval from the UKAS quality manager is required and it must be detailed in the appropriate analysis log sheet.

For example: The performance of newly installed analytical columns on the ion chromatography has a consistently positive bias from the overall mean of results. Although the bias is confirmed to be inherent on the manufactured column itself, and the individual control charts are still shown to be within control, confirmation from the lab manager and UKAS quality manager has to be authorised and logged prior to executing 'split the control limits'.

The option remove from/add back this point to the calculations from the 'Control Chart Actions' menu will not be necessary as the intended protocol for deleting or adding back points to the control chart involve integrating results with an arbitrary character, namely '\$'. This allows calculations of standard deviations for control limits and plotting points on the charts from a series of results to omit unidentifiable numbers (i.e. numbers integrated with \$ symbol).

Add or remove comments. Note that comments reported on a given point will be marked on the control charts as well. Their intended use includes, but is not limited to marking the start of QC reviews, non-conformity log entries, or start of new stock standard solution preparation.

**Chart actions:** Axis/size reset is for reconfiguring the charts displayed.

**Multiple point actions:** The only option of interest is select the subgroup (sample) identifier at which to start the chart. This will allow the user to control how many points to see on the chart at any given time.

**Worksheet actions:** Make subgroups from single column is not necessary. This function is replaced by constructing pivot tables to reformat individual points by grouping them based on run dates as detailed further in appendix 2.

## Constructing a new XBar chart (Batch Mean Measurement Chart)

Test rule violations for the BMMC are:

1. 10 out of 11 consecutive points in a BMMC for an analyte fall one side of the mean.
2. 8 points in a BMMC for an analyte successively rise or fall.

SPC for Excel tab> Variable>Subgroup charts>Select desired chart type (Xbar-R chart)>Fill in information\*>Select OK

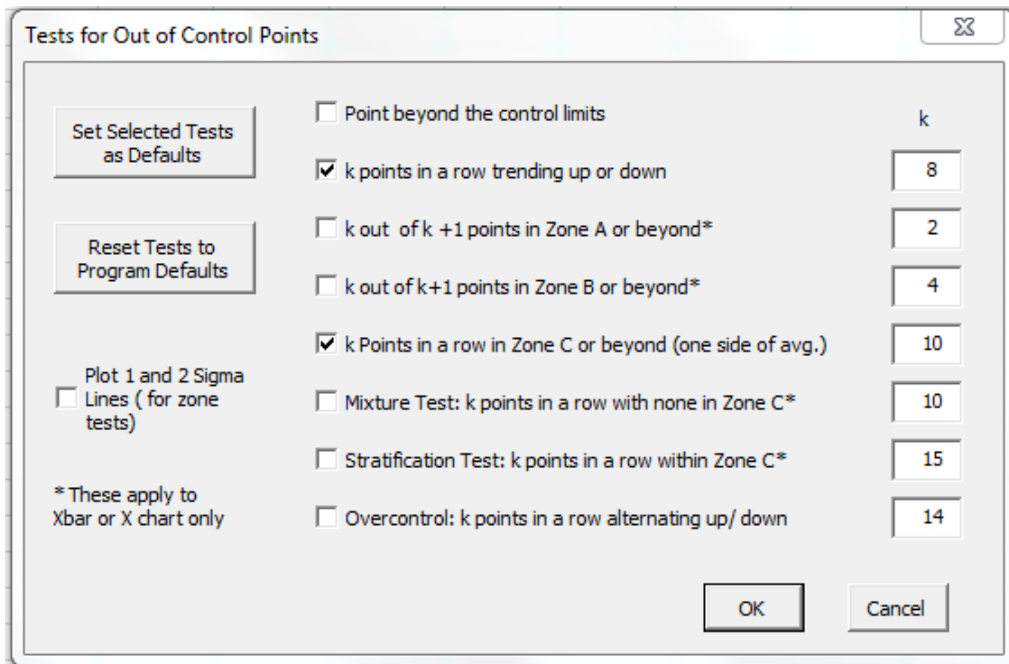
**Figure 12.** Pop up display once the variable for subgroup charts is selected.

\*Further details for filling information below:

**Ranges-** This section requires either sequential numbers or dates from a given column (Subgroup identifiers) and the data array you would like to input, **Chart Input-** Requires name and subgroup size (10 or maximum subgroup used). Selecting the top left result and selecting subgroup size as 10 extends the selection automatically across columns (for a total of 10 columns per row), **and Options-** Crucial sections for constructing the control charts are 'control limit options' and 'out of control tests'.

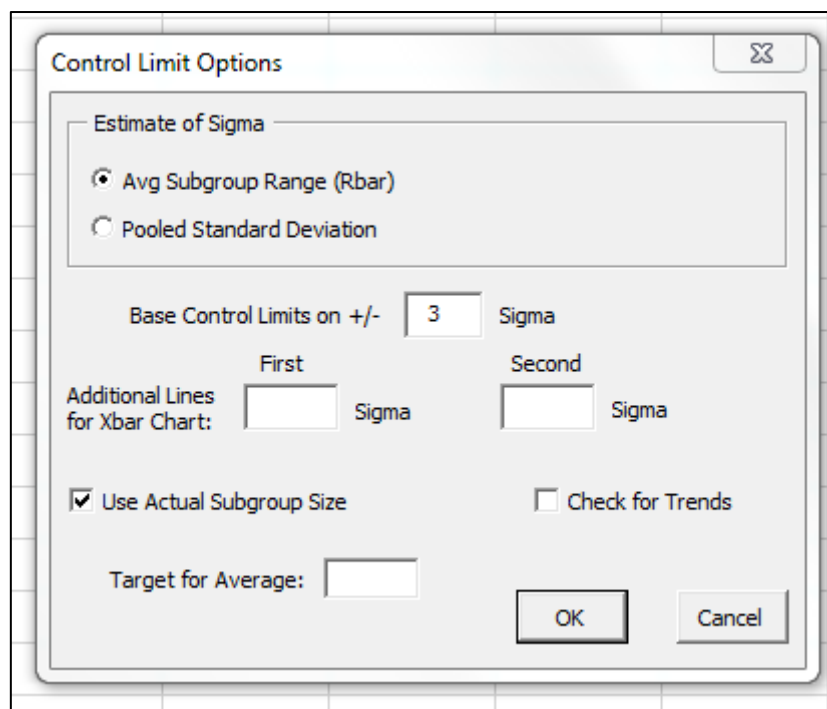
The control tests for BMMC chart are detailed above and should be outlined in an Analytical Quality Control procedure (AGN1.7). To construct the BMMC in SPC:

1. Select out of control tests from the options section which will display what is shown in Figure.
2. Ensure 'Plot 1 and 2 sigma lines (for zones tests)' is deselected. Only select the following test rule violations: 'K points in a row trending up or down (K set to 8)' and 'K points in a row in zone C or beyond (one side of the avg.) (K set to 10)'.



**Figure 13.** Out of control tests for BMMC.

3. In the Control Limit Options pop up, select Avg Subgroup Range (as seen in Figure 14). Ensure 'Check for trends' is deselected.



**Figure 14.** Control limit options setup.

4. Chart location default is to produce chart on a new sheet. Select OK.
5. From the manual control limits section, input the upper and lower specified limits in the UCL and LCL empty cell boxes respectively for the XBar chart.

## Checklist requirements for setting up BMMC control charts

- ✓ Title is set as the analyte name
- ✓ X-axis subgroup numbers are listed as 1,2,3, etc.
- ✓ Y-axis subgroup average response is labelled as (concentration mgL-1)
- ✓ Only have the following limits displayed:
  - Specified limits\* (fixed)
  - Average
- ✓ Default out of control tests
  - 8 consecutive points falling or rising
  - 10 of 11 points above or below the mean

\*Note that the specified limits on the BMMC charts are referred to as UCL (High) and LSL (Low).

## Updating existing BMMC charts

Refer to appendix 2 for details on creating pivot tables. They are pertinent for constructing and updating the BMMC charts. They will enable BMMC charts to have points plotted based on rundates.

### Instructions for updating BMMC chart:

- Once data has been inputted on the sheet containing raw individual points as detailed in the section 'Updating existing Levey-Jennings chart (Individual control charts)', enter the sheet containing pivot tables. Hover over the table array>right click>Refresh.
- This will add the new sets of data gathered from the individual datapoints sheet. In addition, the rest of the pivot tables on the same sheet will also be updated automatically.
- Afterwards, it is a matter of selecting 'update charts' as shown on Figure and updating all charts.

## Appendix 1: Reformatting legacy data in QIA within excel for use in SPC for Excel

Initially the data copied over from the QIA software would be in a different format to what is a required format for SPC for Excel to extract data and construct the charts.

In order to use the SPC for Excel, make sure all data is formatted correctly with the number, date and QC value headings. Ensure any date gaps are filled in as in Figure. Then remove empty rows to produce a data set similar to the functional template shown in Figure which will work with the add-in SPC for Excel.

	Number	Date	QC			Number	Date	QC		
1					1					
2		18/05/2006	12.9		2		18/05/2006	12.9		
3		18/05/2006	12.89		3		18/05/2006	12.89		
4		18/05/2006	12.87		4		18/05/2006	12.87		
5					5					
6					6					
7					7					
8					8					
9					9					
10		24/05/2006	12.88		10		24/05/2006	12.88		
11		24/05/2006	12.88		11		24/05/2006	12.88		
12					12					
13					13					
14					14					
15					15					
16					16					
17					17					
18		16/08/2006	12.88		18		16/08/2006	12.88		
19		16/08/2006	12.89		19		16/08/2006	12.89		
20		16/08/2006	12.87		20		16/08/2006	12.87		
21					21					
22					22					
23					23					
24					24					

**Figure 15.** Addition of date cells is required prior to the use of the SPC for Excel functionalities.

	Number	Date	QC	
1				
2	1	18/05/2006	12.9	
3	2	18/05/2006	12.89	
4	3	18/05/2006	12.87	
5	4	24/05/2006	12.88	
6	5	24/05/2006	12.88	
7	6	16/08/2006	12.88	
8	7	16/08/2006	12.89	
9	8	16/08/2006	12.87	
10	9	09/11/2006	12.9	
11	10	09/11/2006	12.9	
12	11	09/11/2006	12.9	
13	12	29/03/2007	12.87	
14	13	29/03/2007	12.78	
15	14	29/03/2007	12.88	
16	15	22/06/2007	12.88	
17	16	22/06/2007	12.86	
18	17	22/06/2007	12.88	
19	18	21/11/2007	12.87	
20	19	21/11/2007	12.85	
21	20	21/11/2007	12.93	

**Figure 16.** Data table without row spaces.

## Appendix 2: Using pivot table functionality to format BMMC data

### Creating a new pivot table

Using pivot tables allows QC results to be sorted based on calibration run dates instead of having subgroups of ten. In other words, it allows how QIA sorts their data to be similar to SPC for Excel.

How to construct SPC for Excel:

- Insert tab>Pivot table>Table range = all data including headers>New worksheet> OK
- From the new sheet, select the pivot table. From the pivot table fields select date, name, and any analyte. Date=ROWS, Name=COLUMNS, any analyte=VALUES.
- Change value field settings for analyte to average
- Hover cursor over the date column>right click> Ungroup
- Go to design>select do not show subtotals>select Grand totals off rows and columns

### Checklist requirements for setting up pivot table

- ✓ Highlight whole table area including the headers
- ✓ Add an extra row to the selection to ensure new data is added into the table
- ✓ From the pivot table itself ensure:
  - Date is in ROWS, ungroup the dates by right clicking the column with dates
  - Name is in COLUMNS, ensure names are standardised (i.e. no distinct ID's which are only present from a few runs)
  - Analyte is in VALUES, analyte value field settings are set to average
- ✓ Results are set to 3 d.p.

Anatomy of a well-constructed pivot table as shown below Table.

**Table 1.** Pivot table display after constructed correctly.

Average of Chloride	QC01/25	QC04/25	QC07/25	QC10/25	QC13/25	QC16/25	QC19/25	QC22/25	QC25/25	QC28/25	QC31/25 (blank)
24/05/2017	#DIV/0!	2.056	2.054								
25/05/2017		2.066	1.975								
31/05/2017		1.865	1.940								
05/06/2017		2.003	2.120	2.152							
07/06/2017		2.001	1.995								
09/06/2017		2.027	1.997								
12/06/2017		2.001	2.038	2.050							
13/06/2017		1.966	1.962								
15/06/2017		2.099	1.986								
19/06/2017		1.994	2.038	2.016	2.051	1.956					
22/06/2017		1.959	#DIV/0!	1.954	#DIV/0!						
04/07/2017		2.007	2.066	2.022	2.111	2.214					
11/07/2017		2.045	2.037	2.048							
18/07/2017		1.932	1.970	1.992	2.067	2.187	2.178	2.060			
25/07/2017		1.964	#DIV/0!	1.966	#DIV/0!	1.967					
26/07/2017		2.022	1.974	2.019	1.977	2.024	2.052	1.976	2.080		
31/07/2017		2.006	2.007	1.987	2.030						
07/08/2017		1.934	1.929	1.916	1.956	1.966	2.005				
14/08/2017		1.974	1.974	1.948	1.992						
21/08/2017		1.893	1.905								
24/08/2017		1.948	1.904	1.683	1.882	1.911	1.891				
29/08/2017		1.817	1.820	1.837	1.837	1.851	1.846	1.868	1.864	1.866	1.876
31/08/2017		1.961	1.934								
04/09/2017		1.959	1.962	1.941	1.969						
(blank)											

Dates are in one column with the QC data clustered based on run date. There is a blank row (Include row 'subgroup identifier when setting up BMMC chart) and a blank column (Do not include blank column as a subgroup).

