Statistical Process Analysis using NWA Quality Analyst software and Agilent OpenLAB ECM Intelligent Reporter

Application Note

Abstract

Statistical Process Control (SPC) is a well-established element of ISO 9001 certified quality management systems. Northwest Analytics (NWA) Quality Analyst software offers advanced statistical functions to analyze chromatography data system (CDS) result data stored in Agilent OpenLAB ECM. This note describes how NWA Quality Analyst software could be used with OpenLAB ECM and ECM Intelligent Reporter.

Introduction

Quality assurance and quality improvement are important elements of ISO 9000 Quality management systems[1]. Statistical Process Control (SPC), Process capability analysis, process performance analysis, and regression analysis are important statistical techniques helping you not only to achieve planned results but also to continually improve your production and lab processes[2].

While processes operate within specifications they still might be out of statistical control resulting in random out-of-spec situations.

SPC helps identify single event or systemic reasons for deviations and uncover opportunities for process improvements[3].

This is not only limited to manufacturing, chemical, or pharmaceutical production processes, but it can be applied to general lab operation and method validation processes. According to the ISO / IEC 17025: "data shall be recorded in such a way that trends can be detected and statistical techniques can be applied to review Results". SPC can also help laboratory's top management to "conduct a review of the ... testing and/or calibration activities to ensure their continuing suitability and effectiveness"[4,5].

To get the best understanding of laboratory trends, large amounts of data, collected over months or years will provide a higher level of statistical significance. With the Agilent OpenLAB ECM Intelligent Reporter result database analytical quantitation results generated by Agilent OpenLAB CDS or Waters Empower can be stored for several years - across multiple labs and across larger time ranges.

The Agilent Report Template Editor or SQL Server Report Builder allows you to generate e.g. method, instrument and/or compound specific result charts (see figure 1). Microsoft SQL server Reporting Services technology refreshes and publishes web-based reports in an unattended mode.

When developing new processes, or improving or troubleshooting existing processes you need to handle your data in a more interactive way and apply various statistical methods to find the most applicable one. Amongst a variety of software packages for advanced statistics, this note describes how to use NWA Quality Analyst with Agilent OpenLAB ECM Intelligent Reporter. The setup is described in an associated technical note *Connecting NWA Quality Analyst software to Agilent OpenLAB ECM Intelligent Reporter*[6]

Software requirements

Visit http://www.nwasoft.com/products/nwa-quality-analyst to request a free trail copy of NWA Quality Analyst.

Please write to Dana Petrusich (dpetrusich@nwasoft.com) for additional sales information.

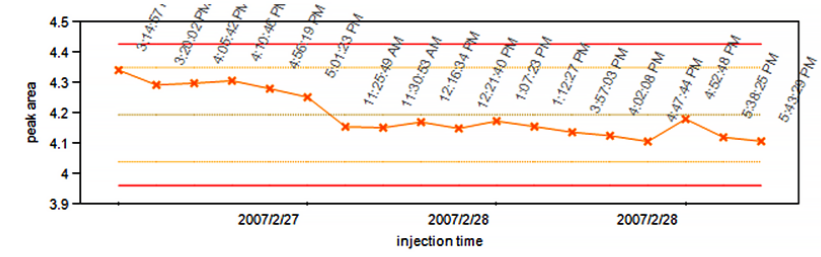
Data backend:

Agilent OpenLAB ECM 3.4.1 with Agilent OpenLAB ECM Intelligent Reporter A.02.0x

Supported CDS systems:

Agilent OpenLAB CDS rev. A.01.03 or higher
Waters® Empower® 2 or 3

Agilent Technologies



Row	InjTime	area	mean area	⊟ evaluation		
				6 σ	trend	imbalance
1	2/27/2007 3:14:57 PM	4.3415	4.1947	-	N/A	N/A
2	2/27/2007 3:20:02 PM	4.2928	4.1947	-	N/A	N/A
3	2/27/2007 4:05:42 PM	4.2985	4.1947	-	N/A	N/A
4	2/27/2007 4:10:46 PM	4.3066	4.1947	-	N/A	N/A
5	2/27/2007 4:56:19 PM	4.2805	4.1947	-	N/A	N/A
12	2/28/2007 1:12:27 PM	4.1557	4.1947	-	-	-
13	2/28/2007 3:57:03 PM	4.1370	4.1947	-	-	7 poins below mean
14	2/28/2007 4:02:08 PM	4.1254	4.1947	-	-	7 poins below

Figure 1. ECM Intelligent Reporter: Individual values control chart with trend and imbalance notification (Shewart rules)

Functionality of NWA Quality Analyst in sum

Complete SPC Charting – Includes variable and attribute control charts, process capability analysis and process based analytics and visualization.

Charting Automation – Procedures easily automated with wizard based "Run File" scripting. Routine charting operations can be called from OpenLAB ECM client with a single icon.

Exception Reports – Reports can be configured to show exceptions based on specification, SPC and pattern rule violations. Includes integrated Assignable Cause / Corrective Action logging.

Industry and Application Specific SPC Modules – Specialized modules such as Multivariate SPC and Stability Analytics add additional capabilities to NWA Quality Analyst.

Examples

Figure 2 shows the result of a process capability analysis. The detected peak area for Anisol in a series of 95 analyses is plotted in a histogram to visualize the distribution type of the result data. A normal distribution is a requirement for applying basic tools of SPC. The diagram shows also the target, and the Upper and Lower Specification limits (USL, LSL) of the process. The capability index C_p is calculated by comparing the width of the specification range with the range of a short term 6σ band. If the ratio is greater 1.5 the process is considered to be "capable" and the potential for the analysis to meet specifications good.

The C_{pk} value relates the closer specification limit to the mean value. It takes into account that processes are not always perfectly centered and bigger differences in C_p and C_{pk} indicate an opportunity for process improvement[3].

Figure 3 shows a control chart based on subgroups of 7 analyses. Individual values and medians of each subgroup are plotted against the number of groups. Since standard deviations become smaller with increasing numbers of samples, the Upper and Lower Control limits (UCL, LCL) are calculated based on a fixed number of samples. They are adjusted if the subgroup contains less than 7 data points to compensate for the expected difference.

Deviations potentially related to a single event ("special cause") are indicated by red dots and tool tips provide information about the violated evaluation rule. Selection of evaluation rules and control limits requires good knowledge of the underlying statistical rules in order to prevent false alarms[3].

Figure 4 combines an individual value control chart with a histogram and a normal probability plot (Q-Q plot). The normal probability plot visualizes the deviations from a theoretical normal distribution of results. Although a histogram of normal distribution may be within specification limits, it does not show the history of data collection and possible trends.

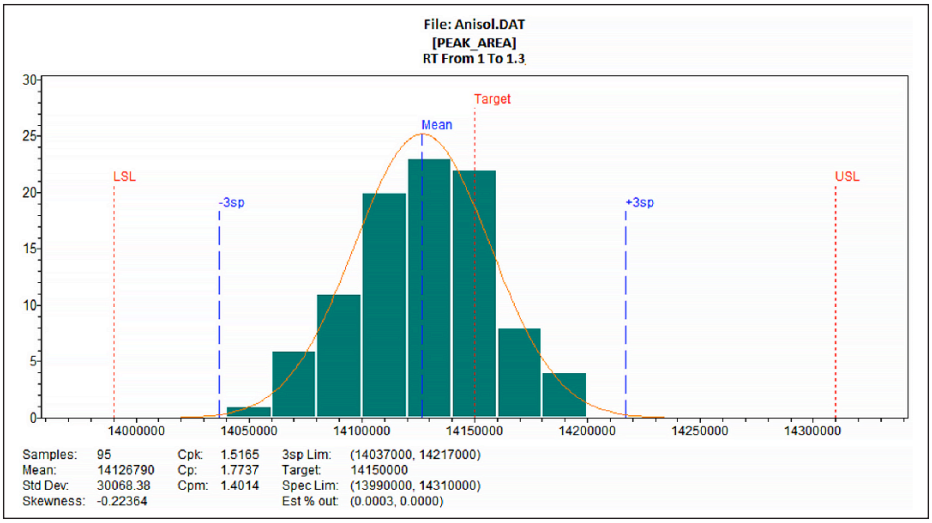


Figure 2. NWA Quality Analyst: Histogram plot of Anisol peak areas showing the distribution pattern of 95 analysis results. The width of the specification range (USL-LSL) in comparison to the calculated 6sp range is a measure for process capability, expressed as capability indices C_p.

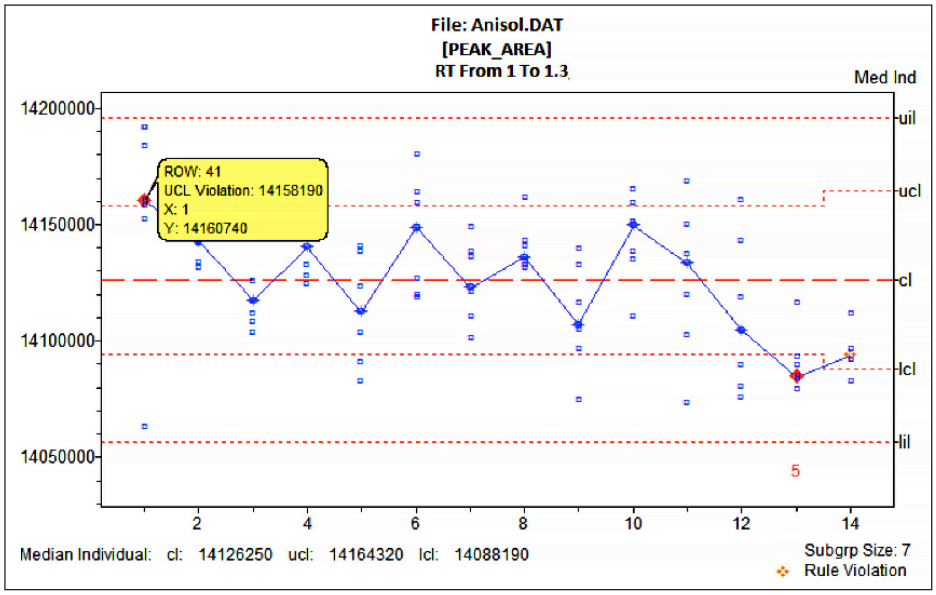


Figure 3. NWA Quality Analyst: Control chart based on the average of 7 individual values for each subgroup. An upper control limit rule violation is indicated by a "Rule Violation" marker. A tooltip shows details of the violation. Implementation of Shewart or Westguard rules are possible, too

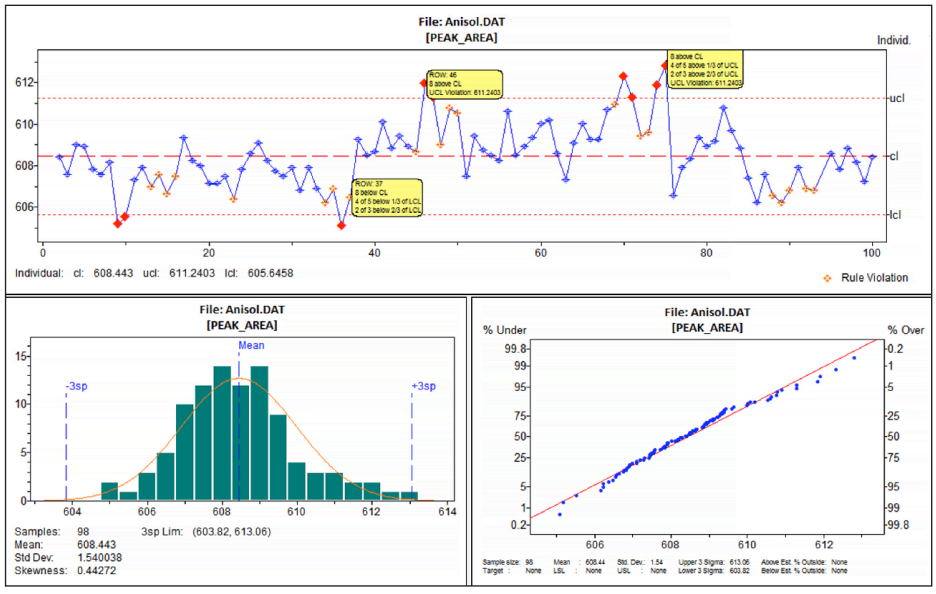


Figure 4. NWA Quality Analyst: Individual values control chart, histogram plot, and normal probability plot can be combined in a single layout.

Integration of NWA Quality Analyst to OpenLAB ECM clients

Generation of pre-defined control charts can be triggered directly from the OpenLAB ECM client. Further automation using OpenLAB ECM Business Process Manager (BPM) is possible. Quality Analyst software operates with various different types of files:

***.DAT files** contain the data used to generate the charts. The *.DAT files could be stored permanently or just temporarily.

***.NWH files**: In case of ECM Intelligent reporter, the database connection and query can be stored in this file type. The NWH file gets generated when saving a new .DAT file.

***.RUN files** are script files that could be used to launch a database connection, call a .DAT file (and the corresponding .NWH file) and generate a chart designed by the Run File Wizard of Quality Analyst

***.NWG** files contain an interactive snapshot of a chart. Storing *.NWH and *.RUN files in ECM is sufficient to preserve a specific database query and chart layout. *.DAT files can always be generated by double-clicking *.NWH files.

Automated chart generation:

By double-clicking a specific .RUN file the Quality Analyst software connects to the database, retrieves the latest data (dependent on the query definition) and generates a single or multiple charts as defined by the run file. This interactive chart can be stored as an interactive .NWG file or in any other graphics format (*.png, *.jpg, *.wmf,*.bmp, *.gif, *.pcx). The chart can be uploaded to ECM to store the history of all control charts.

Interactive chart generation:

By double-clicking a specific .NWH file the Quality Analyst software connects to the database, retrieves the latest data (dependent on the query definition) and shows the data in the Quality Analyst application window.

The application window allows further filtering of the data, modification of the database query and generating all kind of sophisticated statistics and charts.

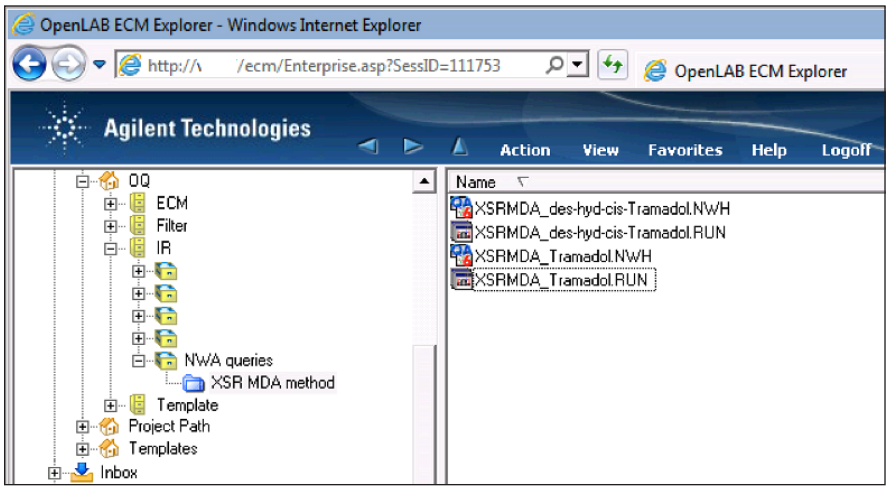
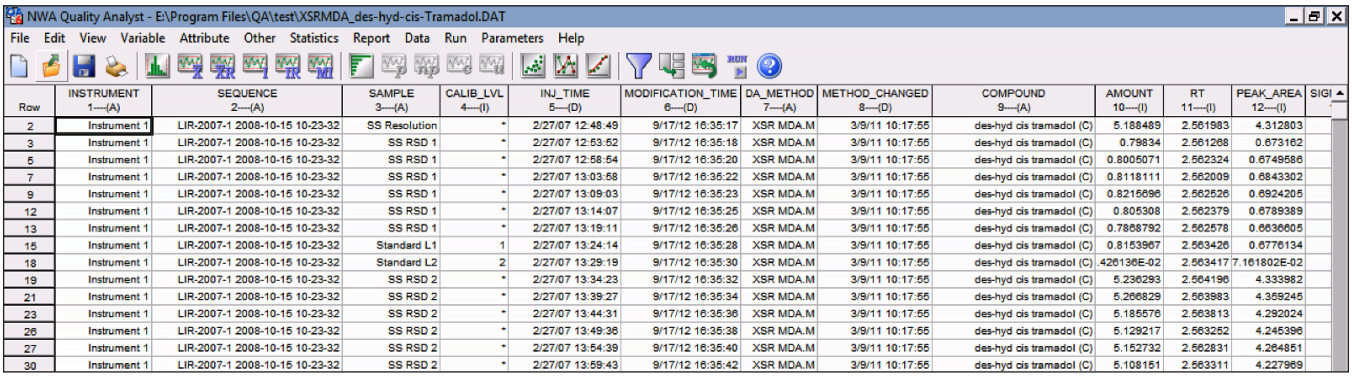


Figure 5. Quality Analyst run files stored in OpenLAB ECM



Row	INSTRUMENT 1---(A)	SEQUENCE 2---(A)	SAMPLE 3---(A)	CALIB_LVL 4---(I)	INJ_TIME 5---(D)	MODIFICATION_TIME 6---(D)	DA_METHOD 7---(A)	METHOD_CHANGED 8---(D)	COMPOUND 9---(A)	AMOUNT 10---(I)	RT 11---(I)	PEAK_AREA 12---(I)	SIGI
2	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	SS Resolution	*	2/27/07 12:48:49	9/17/12 16:35:17	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	5.188489	2.561983	4.312803	
3	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	SS RSD 1	*	2/27/07 12:53:52	9/17/12 16:35:18	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	0.79834	2.561268	0.673162	
5	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	SS RSD 1	*	2/27/07 12:58:54	9/17/12 16:35:20	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	0.8005071	2.562324	0.6749586	
7	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	SS RSD 1	*	2/27/07 13:03:58	9/17/12 16:35:22	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	0.8118111	2.562009	0.6843302	
9	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	SS RSD 1	*	2/27/07 13:09:03	9/17/12 16:35:23	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	0.8215696	2.562526	0.6924205	
12	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	SS RSD 1	*	2/27/07 13:14:07	9/17/12 16:35:25	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	0.805308	2.562379	0.6789389	
13	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	SS RSD 1	*	2/27/07 13:19:11	9/17/12 16:35:26	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	0.7868792	2.562578	0.6636605	
15	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	Standard L1	1	2/27/07 13:24:14	9/17/12 16:35:28	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	0.8153967	2.563426	0.6776134	
18	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	Standard L2	2	2/27/07 13:29:19	9/17/12 16:35:30	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	4.26136E-02	2.563417	7.161802E-02	
19	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	SS RSD 2	*	2/27/07 13:34:23	9/17/12 16:35:32	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	5.236293	2.564196	4.333982	
21	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	SS RSD 2	*	2/27/07 13:39:27	9/17/12 16:35:34	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	5.266829	2.563983	4.359245	
23	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	SS RSD 2	*	2/27/07 13:44:31	9/17/12 16:35:36	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	5.185576	2.563813	4.292024	
26	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	SS RSD 2	*	2/27/07 13:49:36	9/17/12 16:35:38	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	5.129217	2.563252	4.245396	
27	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	SS RSD 2	*	2/27/07 13:54:39	9/17/12 16:35:40	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	5.152732	2.562831	4.264851	
30	Instrument 1	LIR-2007-1 2008-10-15 10-23-32	SS RSD 2	*	2/27/07 13:59:43	9/17/12 16:35:42	XSR MDA.M	3/9/11 10:17:55	des-hyd cis tramadol (C)	5.108151	2.563311	4.227969	

Figure 6. NWA Quality Analyst with query results from OpenLAB ECM Intelligent Reporter

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