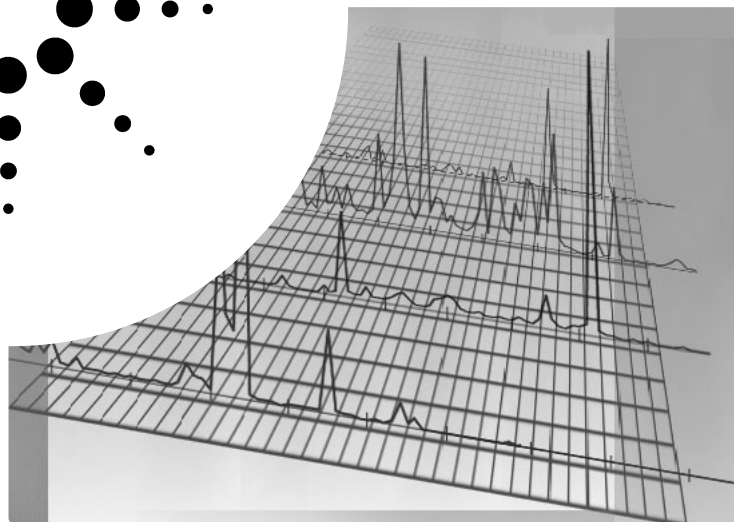


Agilent Cerity Networked Data System for Chemical QA/QC (A.04.03)

Data Sheet



General Description

The Agilent Cerity Networked Data System for Chemical QA/QC (Cerity NDS) is designed for routine QA/QC laboratory environments. It runs on either the Microsoft® Windows 2000® Professional (service pack 2) or Windows XP® Professional. The system can be configured for up to 32 GCs. Up to eight of them can be active at one time.

The software, on CD-ROM, contains extensive online help and tutorials for system operation. The user interface (screens), online help, and tutorials are supplied in nine languages:

Brazilian Portuguese

Chinese

English

French

German

Italian

Japanese

Korean

Spanish

Cerity NDS for Chemical QA/QC controls Agilent 6850, 6890, 3000 GCs, and 35900E A/D using standard LAN communications (TCP/IP) and the 4890, 5890, and M200/Quad GCs using RS-232. Cerity for Chemical controls GC parameters (valves, heated zones, oven temperatures, detectors [with 6890, Cerity supports FID, TCD, ECD, μ ECD, NPD, FPD, and AIB], inlets [with 6890, Cerity supports S/SL, Packed and Cool on Column], cryogenic cooling, signals, electronic pneumatic control [6850 and 6890], sampler operation, etc.) and collects full-range digital signals from detectors.

Hardware

The data system consists of a personal computer (PC) and Agilent software. The hardware is an

IBM-compatible personal computer. Hardware components other than those supplied by Agilent Technologies may require a separate remote cabling system for time-critical events such as injection.

The data system has been tested on Hewlett-Packard (HP) and Compaq PC hardware that conforms to the specifications shown below. Although the software is designed to run on other IBM-compatible hardware, Agilent will not necessarily accept responsibility for defects reported on non-HP/Compaq hardware.

All hardware and peripherals must appear in the appropriate Microsoft Windows operating system Compatibility Lists.



Agilent Technologies

Minimum PC Configuration

- Pentium III (400/450 MHz) with 128 Mbytes RAM (256 Mbytes for four- or eight-GC control)
- 6.0 GB hard drive
- Microsoft Windows 2000 Professional (service pack 2 or higher) or Windows XP Professional. Windows is not included with software.
- Microsoft Internet Explorer 5.5 (service pack 2) or higher
- LAN interface for Agilent 6850, 6890, 3000 GCs, and 35900E A/D.
- RS-232 interface for Agilent 4890D, 5890 Series II, and M200/Quad GCs.
- Ethernet LAN interface (RJ45) connector for PC
- Super VGA display (at 1024 × 768 resolution)

LAN Configuration Requirements

Additional Hardware Required for LAN Instrument Control

- Industry-standard LAN card for the PC. This is standard in every Agilent-supplied PC bundle.
- GC LAN card. This can be ordered as an option to the instrument or separately. Please contact your Agilent representative for details.
- Industry-standard LAN cabling compatible with your network topology.

Twisted Pair

Ethernet twisted pair with RJ45 connectors can be used with a G2402A analytical hub to connect one or more GCs to the PC.

A twisted pair 'crossover-wire' can be used for making a single connection from one PC to one GC without

using a hub. This configuration works only in a single GC situation.

Network Performance

The following network performance was observed using eight 6850 and 6890 GCs generating 200 Hz data and networked on a 10Base-T Ethernet LAN:

- Average network usage of about 4% (400 packets/sec) with peak usage of about 10% (1,000 packets/sec)
- No collisions
- No network errors

200 Hz is the maximum data collection rate for the 6850 GC. Network usage would decrease proportionately with decreasing data collection rates (20 Hz is adequate for most purposes).

Printers

The system operates with most Microsoft Windows-compatible printer directly connected to the computer through a parallel or serial interface or a Microsoft Windows-compatible printer connected through a LAN. Recommended printers are the Hewlett-Packard LaserJet family or, for lower-performance applications, the HP DeskJet family (not recommended for high throughput applications).

Software

Methods and Work Lists

An Agilent data system analytical method describes how a particular separation is performed. It contains all the parameters for GC/sampler control and data acquisition and evaluation, including integration, quantification, and reporting.

A method is developed for a particular instrument configuration (column, gases, inlets, detectors). The sample is logged into the system by entering a sample name. This adds the sample to the database and displays it in the sample summary table. Samples are logged and submitted to a GC work list, which is a queue of samples to be run on that specific instrument. Once in the work list, the sample is run and data is processed by the system.

A “sample mask” can be associated with a specific method. Each sample mask identifies the names of samples that may be run by a specific method. Samples whose log-in names match a mask can be automatically added to the appropriate instrument work list.

While a work list is running, more samples can be added to it and the system will continue to run until it has no more samples in the list. The work list can be paused manually at any time or automatically upon reaching a specified sample. The work list may be re-ordered at any time to allow priority sampling.

System Configuration

The ConnectAdmin program defines the GCs to which the system will connect. ConnectAdmin can store information about 32 GCs in an instruments-available column. The user can control up to any eight of these by moving them to the instruments-enabled column at any time. The software automatically refreshes the enabled/disabled lists and establishes communication to any new GCs added to the list.

Data Model

All system data (including raw data) and methods are stored in a protected database so no data can be overwritten. Sample data, method and instrument parameters are easily archived. Changes to a method are stored as a new version, rather than overwriting the original version. Thus the method used to

generate the results is forever linked to the sample and is available for data recalculation.

Software User Interface

The user interface consists of four main views, one each for viewing Samples, Instruments, Methods, and Reprocess.

Customize User Interface

The Cerity NDS for Chemical QA/QC software allows for very fast customization (less than 1 minute) of the capabilities available for each user. Just click on the capabilities you want available. Your users will no longer have to contend with screens that they never use. This allows the user capability to grow as they become more knowledgeable of the analysis and the Cerity software. Training for new users is also greatly reduced.

Sample View

This view displays a summary table of all samples in the database and their status. Samples may be in a logged, queued, running, or completed state. When a sample run is successfully completed, it can be highlighted in the summary table to show the relevant information in the following sub view.

The **edit view** is for adding samples to the summary table or editing logged sample information. Here the user enters the sample name, sample type, location, user, and any user-defined fields that must be entered into the database.

The **automation view** is for scheduling samples to be run on a regular basis—for example, every 15 minutes. The user can specify the numbers of samples to be run or run them “continuously.”

The **results view** displays the sample results—including peak retention times, areas, heights and peak identification—after the run is complete. A reference

chromatogram can be automatically displayed with the sample chromatogram for easy comparison of results.

The **report view** generates a report of analysis for any completed, highlighted sample in the summary table.

The **instructions view** is a document viewer that presents any file supported by Microsoft Internet Explorer. It can be used to display standard operating procedures, graphical reference chromatograms, or a web site containing relevant information.

Instrument View

The **sample entry view** allows the user to quickly enter samples into the work list, start running the work list, view the real-time plot, and see the instrument status from a single screen. When limits have been set in the calibration table, any sample that is "out of limit" will be highlighted.

The **instrument view** shows the instruments currently connected to the system. Lower-level view show detailed information for the instrument highlighted in the summary view.

The **configuration view** shows the hardware configuration of the connected GC/sampler with parameters such as gases, syringe size, column dimensions, and any connected valving.

The **work list view** shows the sample queue of an individual instrument. This work list can be started, paused, or aborted and the order of the queue can be adjusted to accommodate priority samples. The entire work list can be paused or can be made to pause before processing a specified sample in the list.

The **status view** shows the current setpoints and actual values for the heated zones and flows of the highlighted instrument.

The **real-time plot view** plots the highlighted GC's current signal output over time. The scale of both time and signal can be adjusted easily and can show up to 60 minutes of signal.

Method View

The **method view** is used by the method developer to set up the GC controls, method description, acquisition settings, integration/calibration settings, data display options, and reporting options. All tabs allow the user to create a new method or to save any changes as a new method name. When creating a method the user can create a completely new method, copy an existing method or import a method from the multitechnique Agilent GC ChemStation.

The **instructions view** allows the developer to see documents that the system may present to the user. Any document that is viewable with Microsoft Internet Explorer can be displayed.

The **general view** permits the method developer to link the method to a document to be viewed by the user, add descriptions, start pre- or post-run programs, show the specific GC associated with a method, and edit the method sample mask.

The **acquisition view** allows the user to set the GC flows, temperatures, signals, valve operations and configuration, as well as the autoinjector parameters associated with a particular method.

The **analysis view** sets up the peak identification, integration, and calibration parameters for a method. These are described in more detail in the following data analysis sections.

The **graphic options view** sets up the display and scaling options used when viewing or reporting data from each signal.

The **output view** sets up the data system output. The user can choose to generate the output immediately following a run or after the results are approved. Valid output types are printer, text, HTML, or comma-separated-value file. Specific report components are selected and a file path is specified for the results. Sample results may also be exported to an AIA formatted file.

The supported components are:

- Area percent
- Height percent
- Normalized percent
- ISTD
- ISTD percent
- ESTD
- ESTD percent
- Peak sums (by retention time range)
- Peak groups (by peak name)
- Method listing

To further automate sample processing, users can specify a root file name, then append a date code or an automatically-incremented counter. This avoids overwriting result files.

All reports include a graphic heading, which you can replace with a header of your own design, followed by information on the sample, method, date, instrument, and operator name. The report then shows the processed chromatogram and the user-specified results and peak table.

Reprocess View

This view can be used to reprocess the results with modified data analysis parameters. The data analysis can optionally be saved in a new method version. This view also provides for reprocessing a user-selected group of samples in a single pass. When Microsoft Office 2000 or XP is installed, it provides for spreadsheet statistics and exporting to Excel.

Data Analysis—Integration

The data analysis part of the system contains an integration algorithm that produces a list of retention times and peak sizes. It has these features:

- Integration parameter definitions to set or modify the basic settings for area rejection, peak width, and slope sensitivity
- Baseline control parameters, such as force baseline, hold baseline, baseline at all valleys, baseline at the next valley, and fit baseline backwards from the end of the current peak
- Area summation control
- Negative peak recognition
- Tangent skim processing, including solvent peak definition commands
- Control commands defining retention time ranges for the integrator operation
- Peak baseline allocation on wandering baseline chromatograms
- An initial peak-height parameter to remove noise-generated peaks
- Peak shoulder allocation through the use of second derivative calculations
- User-selectable exponential- or straight-tangent skim mode which is displayed on the integrated chromatogram

In unusual cases where the standard integration baseline is not suitable, the baseline can be modified using the cursor.

Data Analysis—Calibration

Calibration can be as simple as assigning names to the peaks in the calibration table or as complex as assigning separate multilevel nonlinear calibration curves to each peak. The data system allows separate calibration curves for each identified peak.

Calibration Weighting

Individual calibration point weighting may be specified.

- Equal—all calibration points are of equal importance in determining the calibration curve.
- Based on the number of calibrations—the significance of a point on the calibration curve depends on the number of times it has been recalibrated.
- Linear fit—the importance of a point is the reciprocal of the peak size of each calibration level.
- Quadratic fit—the importance of a point is the square of the reciprocal of the peak size of each calibration level.

Curve Type

The calibration curve type may be selected from the following:

- Piecewise linear—a point-to-point interpolation
- Linear—a linear regression fit of the data points
- Quadratic—a quadratic fit of the data points
- Cubic—a cubic fit of the data points
- Exponential—an exponential fit of the data points
- Logarithmic—a natural logarithmic fit of the data points
- Power—a power fit of the data points

Origin Treatment

The origin of the calibration curve may be specified:

- Ignored—the origin (0,0) is not used in the curve calculations.
- Forced—the curve is forced through the origin.
- Connected—a linear segment is constructed between the origin and the lowest calibration point.

Data Analysis—Peak Identification

Peaks are identified by comparing retention times of the peaks in the sample analysis with those in the calibration table.

Individual retention time windows and the use of reference peaks adjusts for retention time drift. Each calibrated compound may have absolute limits for the calculated amount. Results lying outside those limits are indicated on the analysis report. The limits may be used in conjunction with the control samples (defined as part of the automation setup) to provide automatic verification of system performance.

Data Analysis—Quantification

Quantification may be based on either peak area or peak height. Calculations are percent, normalized percent, external standard, external standard percent, internal standard, and internal standard percent.

Programmatic Access to Results

The method developer can designate pre- and post-run programs that are executed as part of the method. These programs can access sample data by accessing either the ASCII text file or the HTML file. For example, a post-run program may traverse the list of integrated peaks and perform a customized calculation.

An example post analysis Visual Basic program is included, with source code, that provides access to report header information, peak information, run logs, and the raw data. This program provides the starting point for custom calculations and reporting.

Documentation

The Certy NDS system comes with extensive online help and tutorials on system operation. When inserting the software CD, the user is able to view or print the following instructions in any of nine local languages:

- Setting up a Certy NDS instrument network
- Adding instruments
- Setting up and calibrating a method
- Running a sample

The data system includes comprehensive, Windows-style, context-sensitive online help with full-text search capabilities. This system gives detailed explanations of every screen and the meaning of the parameters on that screen. The detailed explanations are complemented by graphics where appropriate, and may be printed or copied to the Windows clipboard for incorporation in the user's documentation. The online help also includes procedures for both common and more complex, technique-specific chromatography tasks to help infrequent users ensure they set up the system correctly.

The online help also contains detailed information on system concepts such as data acquisition, integration, calibration, and database management.

Learning the Software

Each Certy NDS system includes task-oriented tutorials. This is the primary learning aid and lets users review topics of interest at their own pace. Each analytical task is divided into a number of clear, guided steps so that users can read, see animated demonstrations of the correct procedure, then practice for themselves.

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