# Using the ChemStore data management module in a ChemStation Plus networked data system to generate sophisticated analysis reports

## Application

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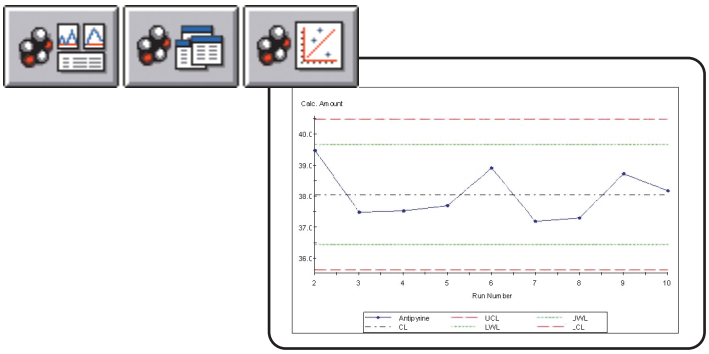


**Abstract**

The Agilent ChemStation base software includes a wide range of built-in report styles and types. For example, it provides standard reports such as area percent (AREA%), external standard (ESTD), internal standard (ISTD), and normalized (NORM) reports as well as system suitability reports and sequence summary reports with statistical evaluation of retention times, areas, heights and more. These standard reports are the topic of a further Application Note[1]. More sophisticated reporting is possible using ChemStore, an add-on software module for the ChemStation base software, thereby creating a ChemStation Plus networked data system. This data storage and management module not only provides for powerful reporting but also offers cross-sample, cross-instrument result review, and second-pass analysis. This application Note describes the reporting capabilities of ChemStore

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## Introduction

Using the add-on ChemStore data storage and management module in a ChemStation Plus networked data system provides the user with database functionality. Whereas the ChemStation base software enables instrument control, data acquisition and analysis, basic reporting and first-pass review, ChemStore provides maximum data protection and integrity for

- organization and management of data in studies
- second-pass review and approval of results
- generation of customized reports
- storage of all related results, raw and meta data in a relational database
- archive and retrieval of data

Before starting with ChemStore reporting, the chromatographic methods, which include integration and calibration parameters, must be set up and tested. For full traceability and change control, all data analysis and re-analysis is done using the ChemStation base software, whereas ChemStore database acts as a data and result management, and review and reporting tool. ChemStore does not allow the user to change integration or calibration parameters – these changes must be done using the Data Analysis part of the ChemStation. This separation of functionality between the two software modules provides both users and auditors with an easy distinction between the tasks of reanalysis and review, thereby maintaining data integrity and capturing all changes in audit trails.

The following sections provide a step-by-step guide for generating ChemStore reports.

## Setting up ChemStation parameters at sample entry before analysis execution

Before you send data to the database, we recommended doing the following steps.

**1** Set up the chromatographic method as well as the integration and calibration tables[1].
**2** Set up the ChemStation sequence table, including correct entries for the sample type, number of injections, and so on[1].
**3** Set the ChemStation report type appropriately. Only those results that are processed in the ChemStation report are transferred automatically to the database. For example, if you want to generate a system suitability report with ChemStore, you must select the report type *Extended Performance* in the ChemStation[1]. In the example described in this note only a subset of this data, including tailing factors and theortical plates, is used to calculate the ChemStore system suitability report, which is a built-in report template. These calculations might only be required for the system suitability samples, for examples, at the beginning of the sequence. Therefore it may be necessary to set up different methods – containing different report types – for samples, calibration standards and control samples. This will depend on the indiviual reporting requirements.

Note that the amount of result data transferred to the database is dependent on the report style selected in the ChemStation chromatographic/evaluation method, the *.M file.

## Setting up ChemStore

Set up a study in the ChemStore review client by choosing *Create Study* from the *Administration* menu, and define storage conditions, users who should have access to this study, and if required, custom field values. When you have set up a study, go to the ChemStation *Method and Run Control* screen and choose *Sequence Setup* from the *ChemStore menu*, see figure 1.

**1** *Click Transfer Settings* to configure the data transfer, report style and destination. This example transfers data after each analysis and uses an existing built-in report template *Compound Amounts Report* , which is printed at the end of the sequence.
**2** Click *Select Study* to select the study destination for data and results from a list of all available studies.
**3** Click *Custom Field Values* to set data entry into optional custom fields.

When you have set these ChemStation and ChemStore sequence parameters, you can start the ChemStation sequence. Data and results are transferred automatically to the selected study into the database. At the end of the sequence the ChemStore report is printed using the selected report template.

## ChemStore reporting tools

ChemStore has three reporting tools; print actual window, advanced comprehensive reports using built-in report templates, and custom reports.

### Print actual window

Printing of the actual window is quick and easy and is done from the main menu. The full content of the window is printed on a maximum of two pages – one page for tabular results and one page for charts or chromatograms. This printing tool offers a quick *snapshot* paper copy of your current data set. This can include the trend chart visualization of your results, demonstrating a drop in resolution of your column and initializing a column change, for example.

This functionality also allows you to export easily the contents of the actual window – tabular results can be exported to Microsoft Excel and graphics can be copied to the clipboard.

### Advanced comprehensive reports using built-in report templates

- Instrument and run report with chromatograms, tables and charts
- Sample summary report
- Compound summary report
- Peak details report
- Kinetics report
- System suitability report

### Custom reports

Custom reports enable combinations of any ChemStore data, including statistics, audit information, cross-sample trend charts, and sample or compound details in one comprehensive report. Custom reports are created either by modifying a built-in template or by starting from scratch.

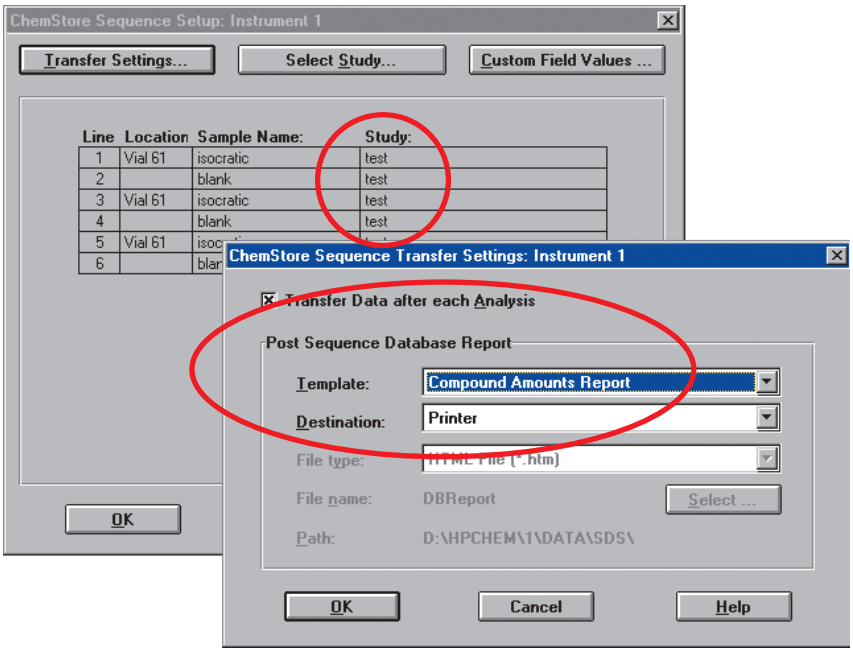



**Figure 1**
**Set up of data transfer and reporting in ChemStore, showing the selected study and the selection of report format and out put**

## Report setup and configuration

ChemStore always creates reports based on a given set of data. This data set is either defined through the ChemStation sequence, when the ChemStore report is generated at the end of data acquisition, or it is defined through the database query.

### Selection of data files for reporting – querying the database

We recommend using data files from an existing study and to modify and create templates using this data set. To start a report first a query must be created. This is done on the ChemStore Review Client by choosing Create Query from the File menu. Creating a query can also be done using the appropriate icon, see figure 2. Clicking the query icon displays the *Query Builder*. Different selection criteria can be chosen and easily combined to narrow down the query output to the desired data set, for example, based on the study name, on sequence file names, on raw data file names such as shown here, on injection volumes, or on acquisition date, and many more. When you have selected the criteria for the query, you retrieve the data by simply clicking *Retrieve* in the *Query Builder*.

### Selecting the overview window

The ChemStore user interface is divided into task-oriented views, as shown in figure 3. The views display either tabular result data or graphical data such as chromatograms and spectra or customizable trend charts.

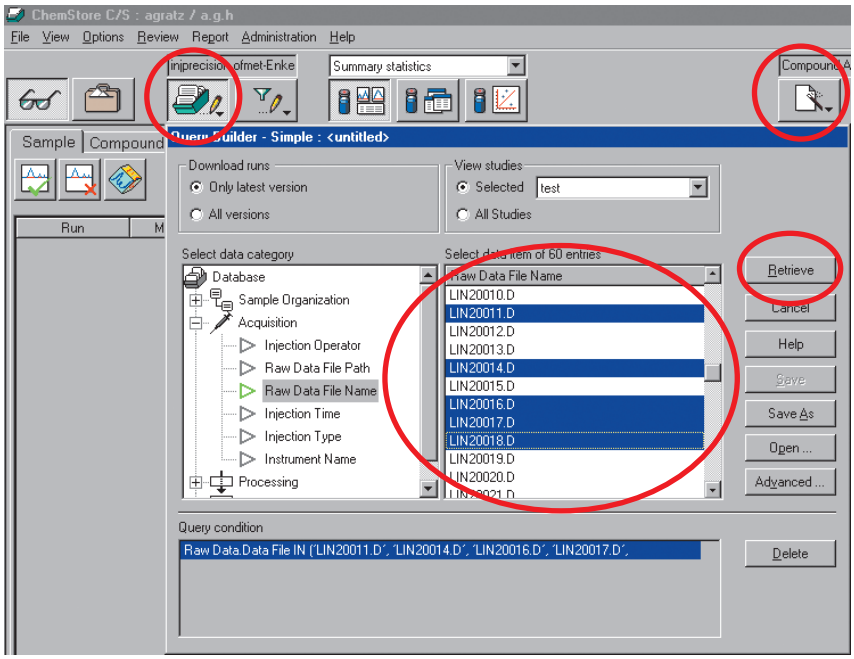



**Figure 2**
**Building a query**
**1. Create a query**
**2. Select data files**
**3. Retrieve data files**
**4. Start report selection and editing**

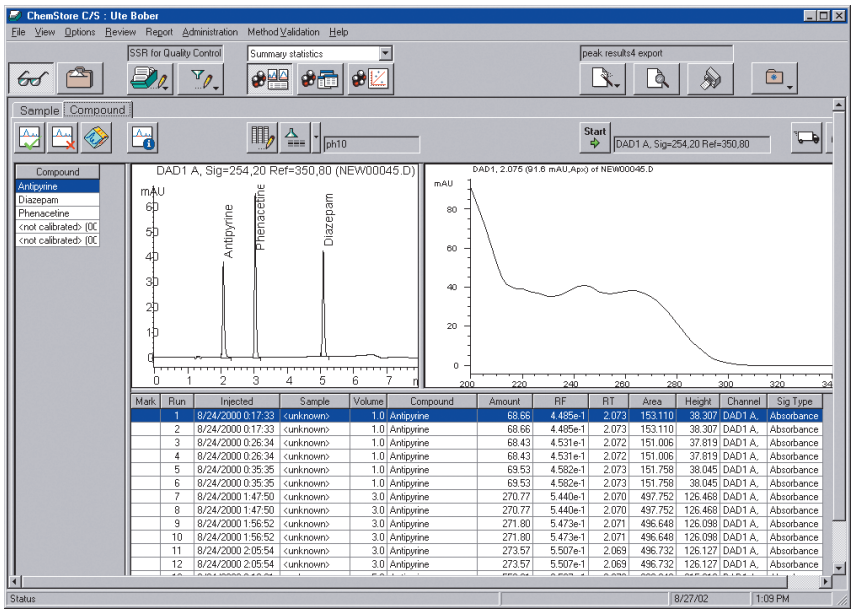



**Figure 3**
**The ChemStore user interface, in which the graphical sections display the chromatogram and spectrum of the highlighted compound**

ChemStore allows the user to define the interface to suit individual requirements. Each user can define their own interface in terms of data display, statistical results, and size and separation of the display. ChemStore has three predefined views.

- Sample-based information and results or individual compound results can be chosen for review using the tabs shown in figure 4.
- Results overview with chromatogram and spectra, results table or trend charts can be selected using the icons as shown in figure 5
- Additional statistical result calculations for summary and regression statistics are available for result tables.

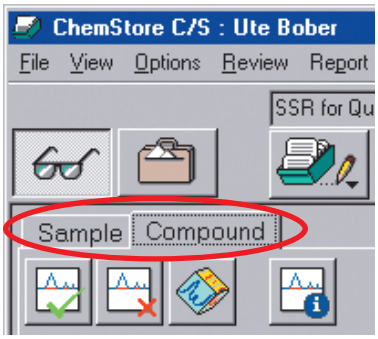



**Figure 4**
**Sample and Compound tabs**

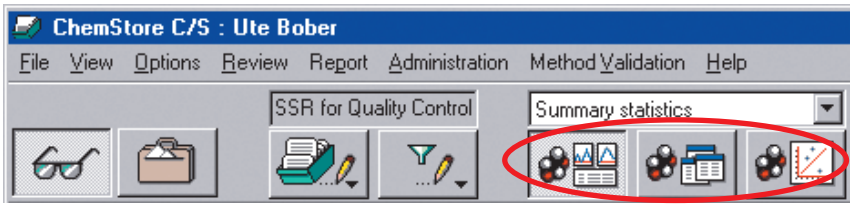



**Figure 5**
**Sub-views for result overview, tabular results and trend charts**

### Configuring the results table

ChemStore displays two tables (see figure 3):

- The table at the left side of the overview window is not configurable because it displays the list of runs or compounds that were retrieved by the query. For the sample view this list includes the actual run number, approval and archive status, and the current result version. In the compounds view the list includes all compounds according to the ChemStation calibration.
- The other table is the result table. This table must be configured using either the icon or by choosing *Columns-Define* from the Options menu as shown in figure 6.

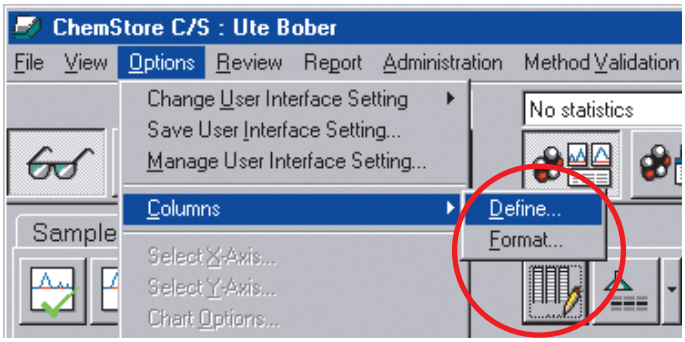



**Figure 6**
**Defining columns through the menu bar or smart ion**

Note that each view has an individual table configuration, thereby requiring the user to repeat the table setup for each view under consideration. Once configured, all tables can be saved for later reuse with the *Save User Interface* command. Each user logging on to ChemStore will find their individual user interface configuration. It is saved with the user's logon details and displays on any client as soon as the user logs on to the database. Once a user interface has been designed and saved, it can be assigned easily to any other user.

The result table is configured similar to the query builder. The user selects the result data from a list of all available results. In addition, each table column can be formatted individually as shown in figure 7. Additional calculations on each column can be configured using the Expression button. This allows, for example, to calculate relative retention times based on one reference.

When the interface has been configured, the user can select *Print View* to get an immediate printout of the contents of the actual window. For advanced reports, the user can set up custom reports tailored to their individual needs.

## Report setup

### Using built-in report templates

ChemStore uses a runtime version of Microsoft Access to generate reports. This offers access to the powerful tools of database reporting. However it also adds some complexity to the report configuration compared to ChemStation reporting. ChemStore therefore includes a set of built-in report templates that are ready to use and do not require any interaction with the report generator. The user simply selects the report template from a list of available templates and starts reporting (see figure 8) by sending the data either to a file or to the printer.

### Setting up custom reports – Report template generation step by step

After loading the data files, the user can print the results using the print functions as described in previous sections. Alternatively, the modification of an existing template or creation of a new template can begin.

### Step 1: Definition and layout of a new report template

If the user is not familiar with report editors, we recommend starting with modifying an existing report template, for example, the built-in *Compound Amounts* Report template. A good strategy is the following:

1 Let data be evaluated by one or several existing report templates.
2 Note the required modifications (this might include modification of the ChemStation report type, to provide the results needed for the selected ChemStore report)
3 Classify the modifications as:
- another column to an existing table
- different selection criteria for an existing table or chart
- different setup for the x and/or y-axis of charts
- a new table
- a new chart

This procedure can be repeated for several existing report templates. Elements from different report templates can be combined and saved as a new customized template.

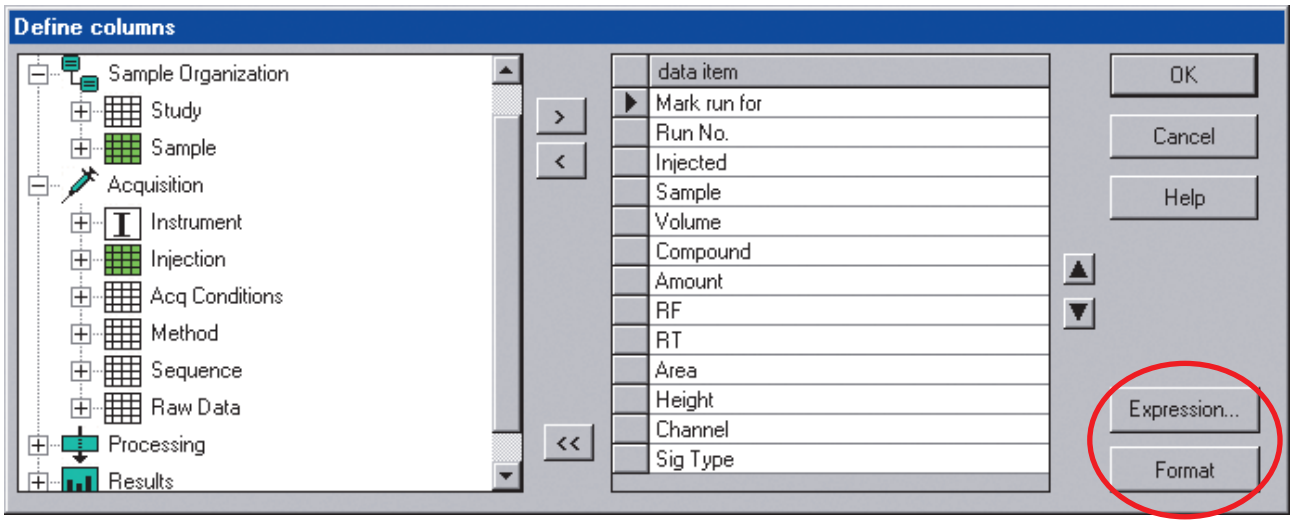



**Figure 7**
**Result tables setup, table column formatting and definition of expressions for custom calculations**

**Step 2: Analyze actual report from a built-in report template**

Data-file retrieval, as described in an earlier section, is required before you can start managing, creating and editing reports. Let's assume that you want to select the report template *Compound Amounts Report* from the existing report templates (see figure 8). In this example the data from the study *Quality Control* is used. Having selected this report template, report generation and print out of the report is done by clicking the print icon.

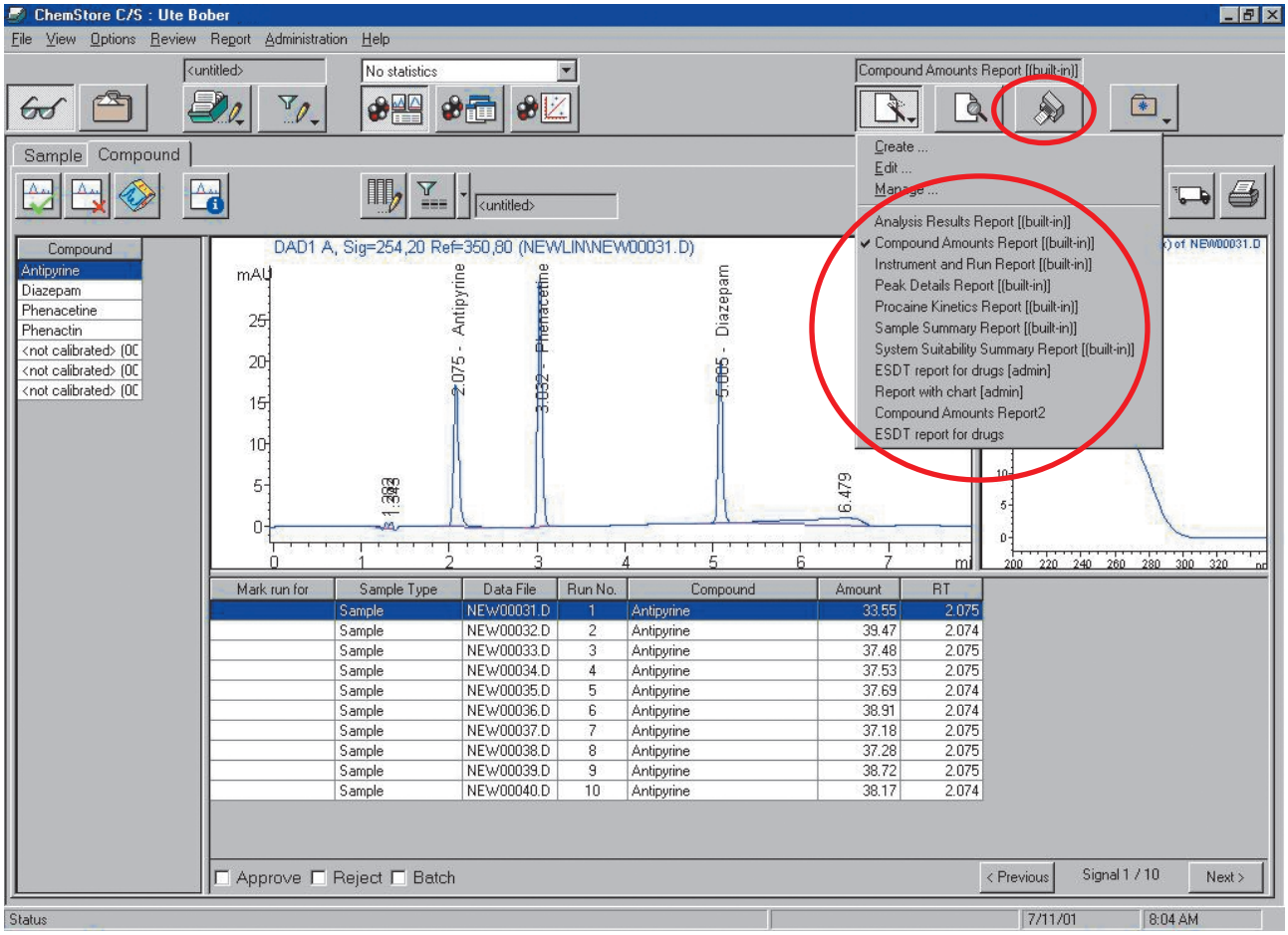
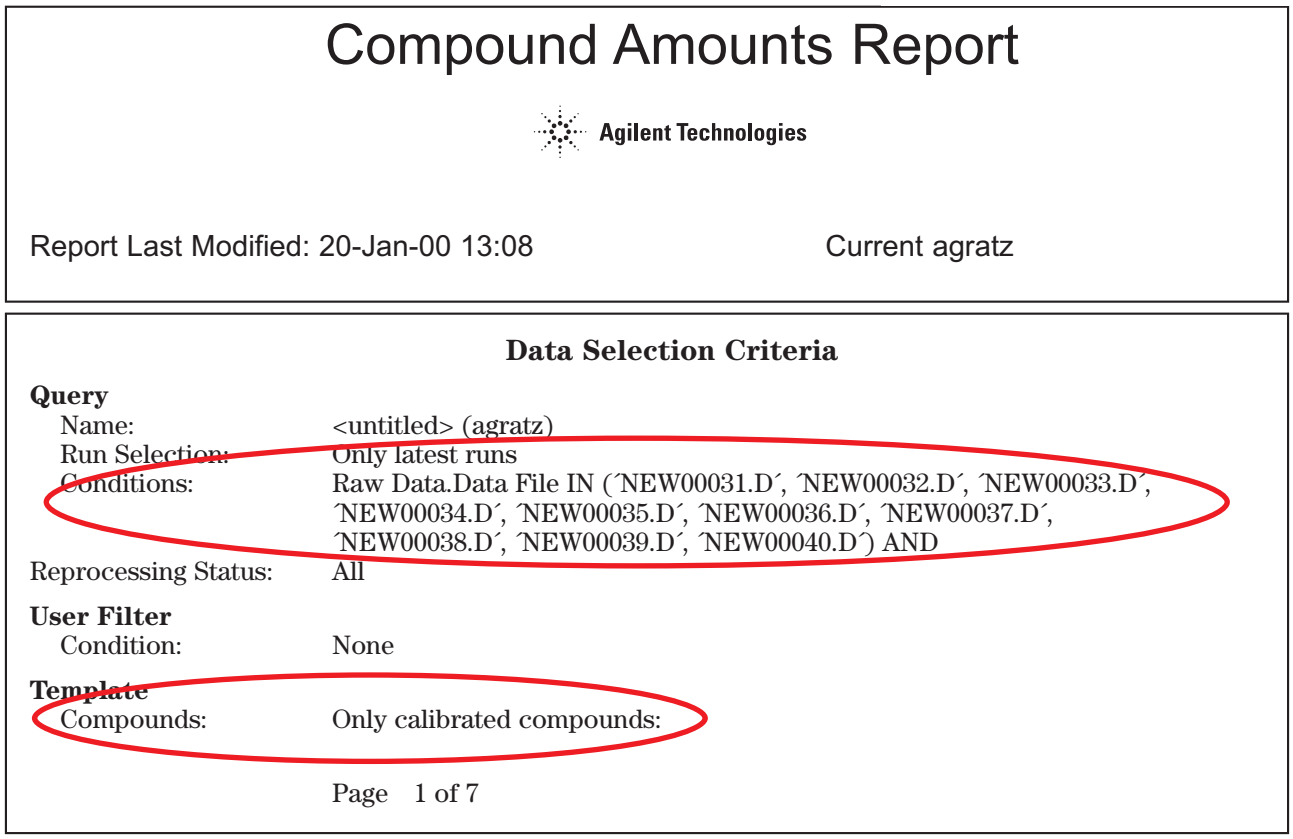



**Figure 8**
**Selection of report template for printing, showing the print icon and the built-in reports (including two user-created report templates at the end of the list)**

**Report examples**

Figure 9 shows the first page of the report, which contains a total of seven pages for the three analyzed compounds. Only the results obtained for antipyrine are shown. The first page contains the header and the selection criteria that were used in the query. In this case the raw data file names were the selection criteria. Further selection criteria were that only results for calibrated compounds should be printed. No other filters or further criteria were used.

On the next report page, the results for antipyrine are printed as a compound table, see figure 10. This type of table contains information about the study name, the chromatographic method used, the compound name and the table with calculated qualitative and quantitative data for antipyrine. The table comprises seven columns that contain run number, sample name, data file name, retention time, peak area, peak height and amount. For the peak time, area, height and calculated amount the precision is calculated and printed at the bottom of the corresponding column.



Compound Amounts Report

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Report Last Modified: 20-Jan-00 13:08 Current agratz

**Data Selection Criteria**

**Query**

| | |
|---|---|
| Name: | <untitled> (agratz) |
| Run Selection: | Only latest runs |
| Conditions: | Raw Data.Data File IN (´NEW00031.D´, ´NEW00032.D´, ´NEW00033.D´, ´NEW00034.D´, ´NEW00035.D´, ´NEW00036.D´, ´NEW00037.D´, ´NEW00038.D´, ´NEW00039.D´, ´NEW00040.D´) AND |
| Reprocessing Status: | All |

**User Filter**

| | |
|---|---|
| Condition: | None |

**Template**

| | |
|---|---|
| Compounds: | Only calibrated compounds: |

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**Figure 9**
**First page of compound amounts report, showing query and compound selection criteria**

# Compound Amounts Report

Study Name: test Instrument Name: Instrument 1
DA-Method: C:\HPCHEM\1\METHODS\LINI22.M
Compound Name: Antipyrine

| Run No. | Sample | Data File | Peak Time | Peak Area | Peak Height | Calc. Amount |
|---|---|---|---|---|---|---|
| Data Path: | C:\HPCHEM\1\DATA\NEWLIN\ | | | | | |
| 2 | <unknown> | NEW00032.D | 2.074 | 72.280 | 17.981 | 39.47 |
| 3 | <unknown> | NEW00033.D | 2.075 | 68.471 | 17.050 | 37.48 |
| 4 | <unknown> | NEW00034.D | 2.075 | 68.568 | 17.082 | 37.53 |
| 5 | <unknown> | NEW00035.D | 2.074 | 68.872 | 17.145 | 37.69 |
| 6 | <unknown> | NEW00036.D | 2.074 | 71.200 | 17.729 | 38.91 |
| 7 | <unknown> | NEW00037.D | 2.075 | 67.894 | 16.916 | 37.18 |
| 8 | <unknown> | NEW00038.D | 2.075 | 68.090 | 16.981 | 37.28 |
| 9 | <unknown> | NEW00039.D | 2.075 | 70.836 | 17.656 | 38.72 |
| 10 | <unknown> | NEW00040.D | 2.074 | 69.777 | 17.379 | 38.17 |
| Mean | | | 2.074 | 69.554 | 17.324 | 38.05 |
| Std. Dev. | | | 0.00051 | 1.55488 | 0.38065 | 0.8131 |
| RSD | | | 0.02 | 2.24 | 2.20 | 2.14 |
| Overall Mean | | | 2.074 | 69.554 | 17.324 | 38.05 |
| Overall Std. Dev. | | | 0.00051 | 1.55488 | 0.38065 | 0.8131 |
| Overall %RSD | | | 0.02 | 2.24 | 2.20 | 2.14 |

**Figure 10**
**Second page of compound amounts report, showing compound Table with selected header, qualitative and quantitative data and statistics**

A compound chart is included on the second page, see figure 11. Here, the amount is plotted against run number and the mean value, the upper and lower warning limits and the upper and lower critical limits are drawn. The user can define these values.

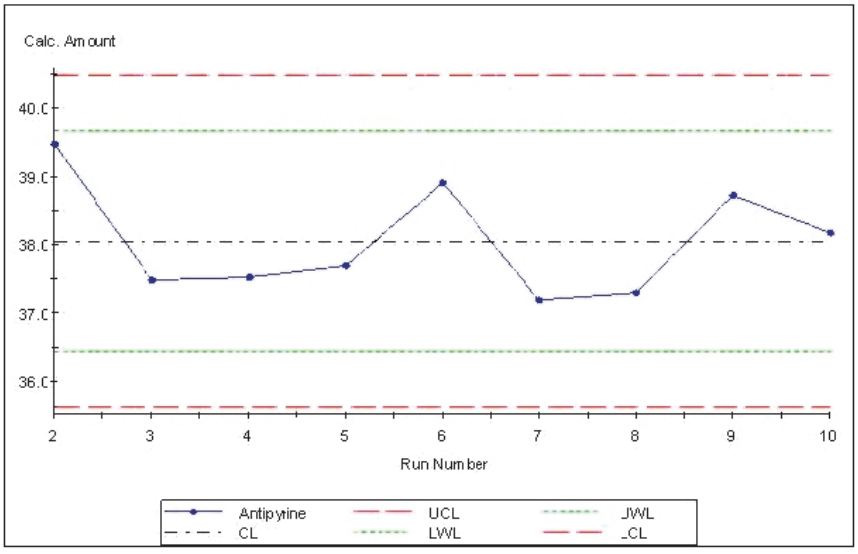



**Figure 11**
**Chart of amount antipyrine per run in compound amounts report, showing mean value, upper and lower warning limits, and upper and lower critical limits**

**Step 3: Modifying an existing element in a built-in report to generate a custom report**

If you want to change the limits for the compound chart, click the report icon again and select *Edit*. To display the Report Editor, see figure 4. The report template for the *Compound Amounts Report* is started as shown in figure 12. The report elements are shown at the left side. If a report element is highlighted, the context-related menu for editing and changing this element appears at the right of the screen.

To change the limit settings for a chart, highlight the item *Compound Chart* under *Data Section*. Choose *Options* to display the menu for limit settings, see figure 13.

Here you can change the expected mean value and the limit settings. In the example, the mean value was set to 38 ng and the upper and lower warning level to 1σ deviation from the mean value. The upper and lower critical limit was set to 2σ deviation from the mean value. Instead of using a specified value for the center line, the calculated mean value can be selected. Having changed the parameters, the report template can be saved under a new name and can be used for further reporting.

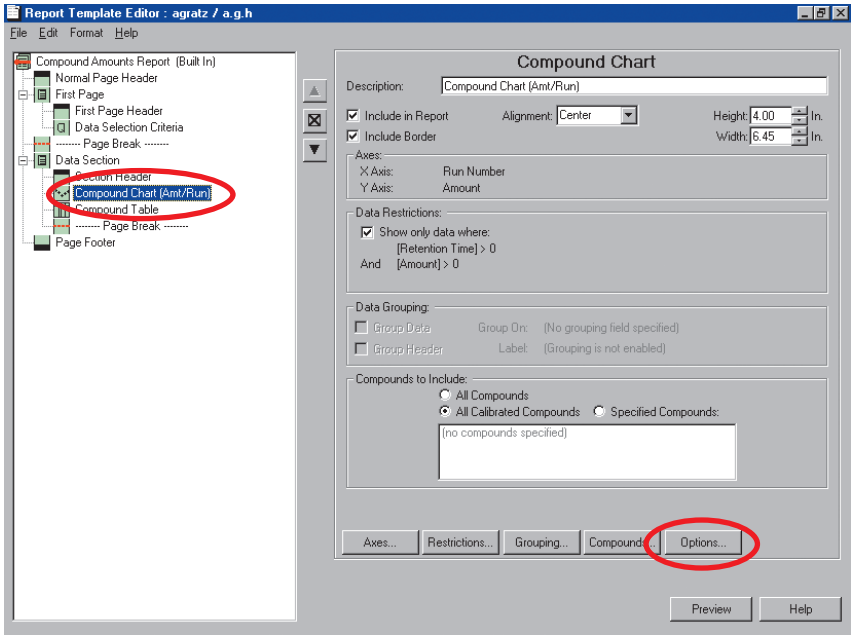



**Figure 12**
**Report Template Editor, showing the template for the compound amounts report – if a report element is highlighted, the appropriate menu for editing and changing parameters for this element appears. Use the Options button to display the menu for limit settings.**

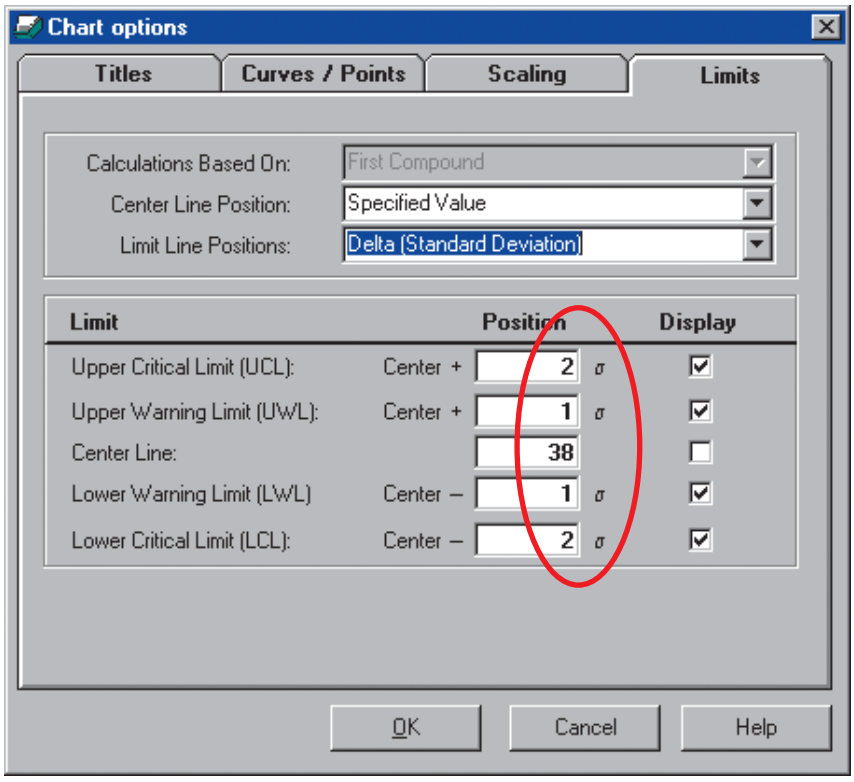



**Figure 13**
**Setting chart parameters – the mean value is specified to be 38 ng, the upper and lower warning level is set to 1% deviation from the mean value, and the upper and lower critical level is set to 2σ deviation from mean value**

**Step 4: Adding a new data element to an existing template Adding a run table**

If a built-in report template does not contain the information needed, a new report element must be added. Select the report section for the addition of the element. Choose *Insert Data Element* from the *Edit* menu, see figure 14. A section header, chart, table, chromatogram and spectrum, print out of selection criteria, and a page break can be inserted. In this example the insertion of a table was selected.

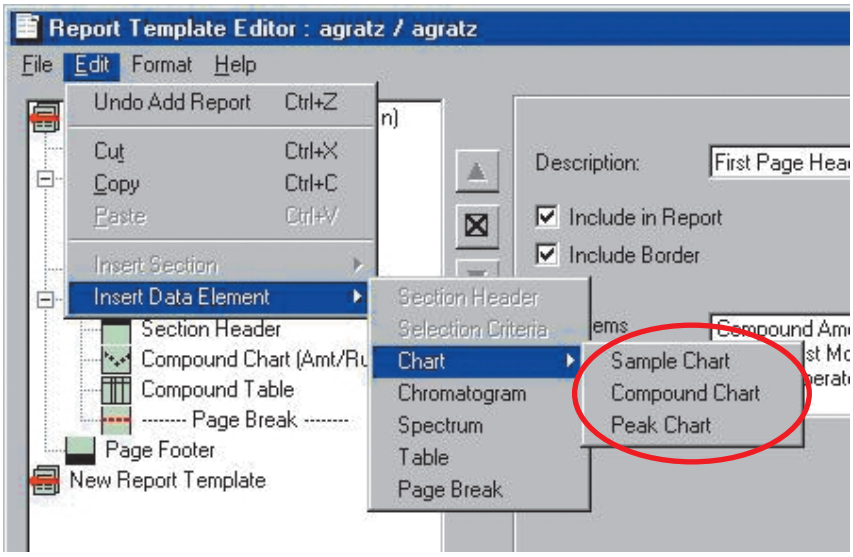



**Figure 14**
**Inserting data elements such as tables and charts**

Several different table types can be added, see figure 15, related to the injection, run, signal, compound, peak, column configuration, instrument components or audit trial. This example explains in more detail how to setup a run table.

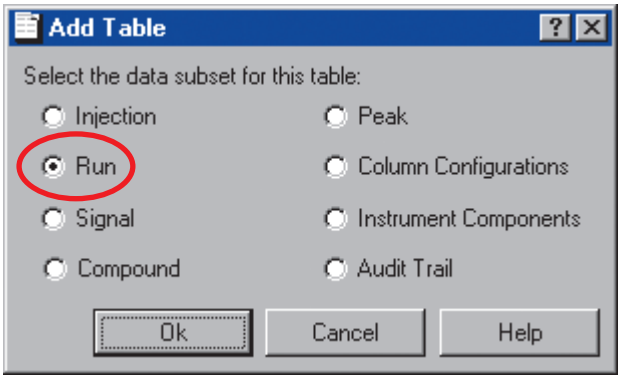



**Figure 15**
**Adding a table – by selecting Run, a result table can be created that contains information related to each run**

All tables contain default columns that are shown at the top of the run table menu, see figure 16). To add or to remove columns, click *Column*.

In figure 17, *Sample Type* has been selected as an additional column. Adding and removing columns is done using the arrows in the center of the menu. Choosing OK confirms the change, which is applied to further reports. The column order can be rearranged using the arrow buttons.

**Step 5: Using logical elements such as grouping or restrictions to generate statistics and overview information**

It is often required to reorganize result data in multiple ways, according to both chronological criteria (such as list of injections) and logical criteria (such as sample type, user name, and so on) instead of a pure sequence-based organization of results. ChemStore provides the following tools to organize data logically.

- Restrictions
- Grouping
- Summaries (for statistics)
- Compound-based filtering of reports

The following examples show how these parameters influence results.

**Restrictions**

An example task would be to create a table with default compound table columns, listing only those samples that contain the compound Antipyrine and thereby avoiding empty and nonsensical lines. Statistical results for all repetitive injections of the same sample are required. In ChemStore reporting terms, this means setting up a new

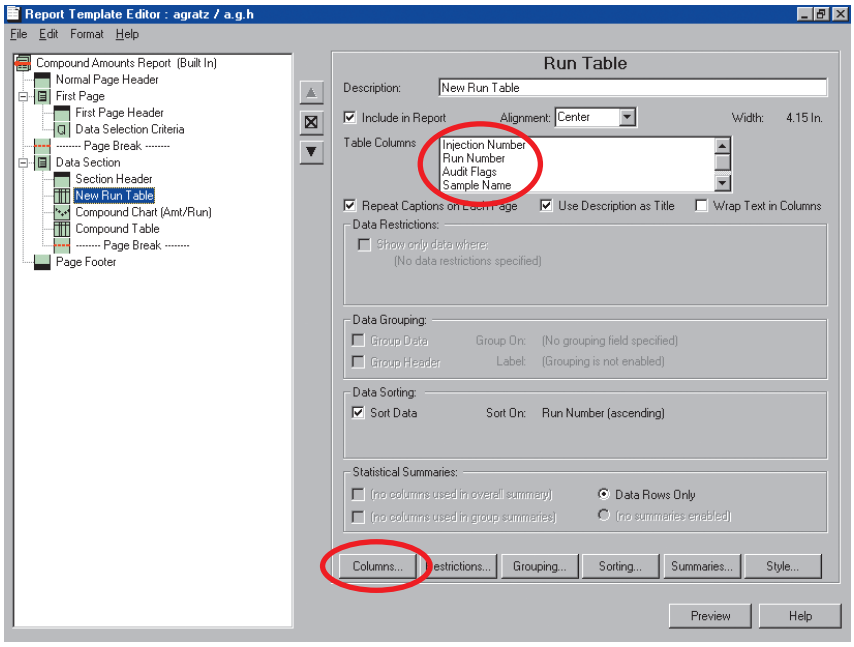



**Figure 16**
**Set up of run table, showing default columns in a run table and addition of a column using the Columns button**

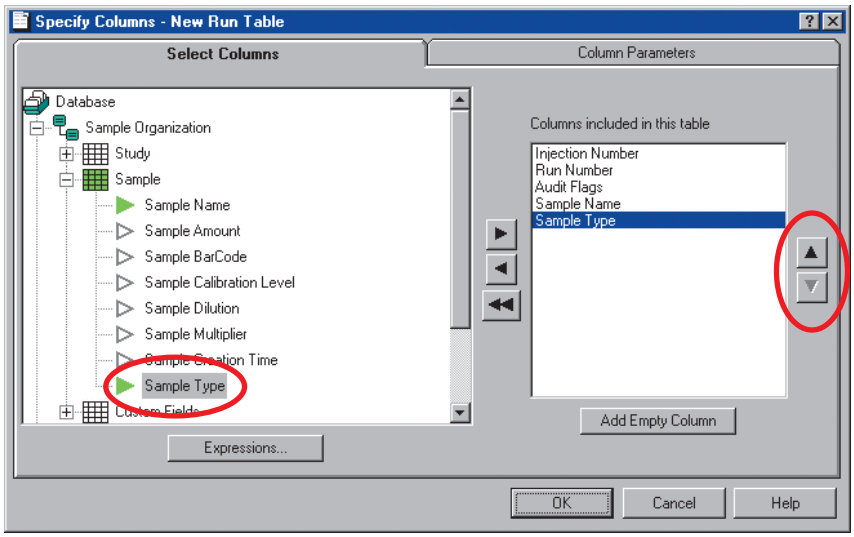



**Figure 17**
**Sample Type has been added as a new column in the run table**

compound table, which should contain the same columns as the built-in *Compound Amounts Report*. Statistical data should be calculated across files with the same injection volume and only for compounds with amounts greater than zero and where the sample type is *Sample*. The Restriction, Grouping and Summaries parameters need to be set up, see figure 18.

**1** Add a new table to the report by highlighting Data Section in the report template and then choose Insert *New Data Element* > *Table* from the *Edit* menu and check *Compound Table*.

**2** Filter the compound data according to the restriction criteria by clicking *Restrictions*, which displays the screen shown in figure 19. In this example the results should be restricted to those runs that include the target compound Antipyrine, and standard or control runs should be excluded. To restrict the information on the compound table, select *Amount*, *Sample type*, and *Compound name* from the available fields and add them to the right side as base restictions.

**3** To each of these base restrictions, data restriction must be added, for example, the *Amount* should be greater than zero. The *Sample type* should always be *Sample* and the *Compound name* should always be Antipyrine. The effect of these settings will be that the compound table will only contain data for Antipyrine, if the *Amount* is greater than zero and if the *Sample type* is *Sample*. Therefore, no calibration runs or control samples will be included.

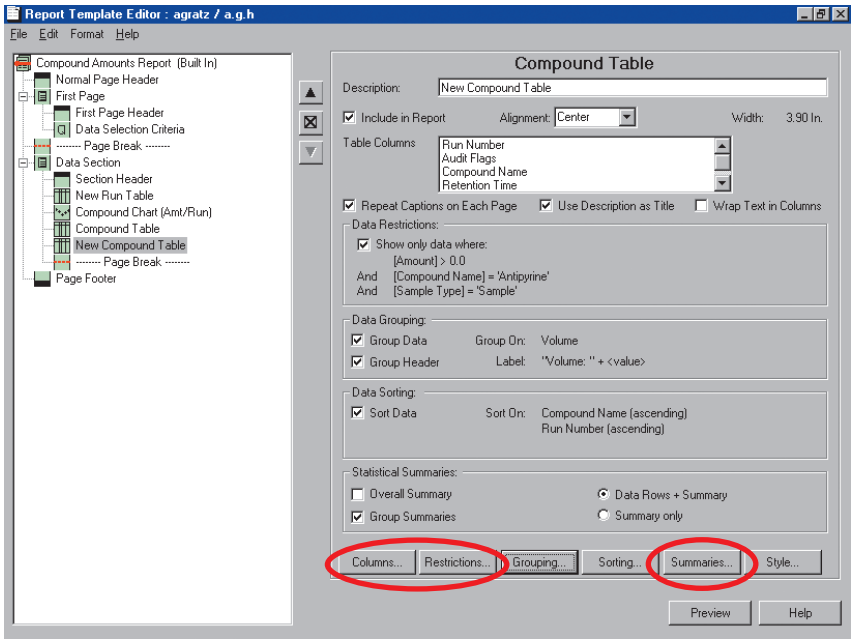



**Figure 18**
**Compound table screen**

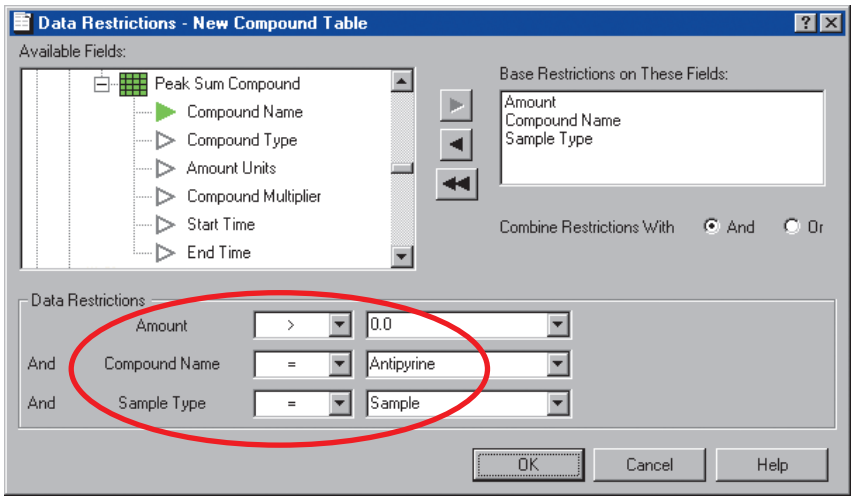



**Figure 19**
**Restriction of table content so that the compound table only contains data for Antipyrine, when the Amount is greater than zero and when the Sample Type is Sample**

### Grouping

In the *Grouping* tool, criteria for the statistical evaluation of the compound table are set, see figure 20. In this case, *Volume* is selected from the available database fields. This means the precision for retention times and amounts will be calculated for those runs with the same injection volume.

### Statistical summaries

In the *Summaries* tool the calculation procedure for the statistic can be selected. Several calculation procedures are available such as mean value, standard deviation and relative standard deviation, see figure 21. Statistical calculations can be applied to all table data or more granular on each group of data as set up with grouping.

### Compound-based filtering of reports

So far the different selection tools for charts and tables have been described. ChemStore also includes a high-level filter for compounds that applies to all data sections and allows users to select the compounds to be included in the report. ChemStore offers four options:

- All compounds
- All calibrated compounds
- Those specified at run time
- Specified compounds (manual restriction to compounds of interest from a list of all available compounds)

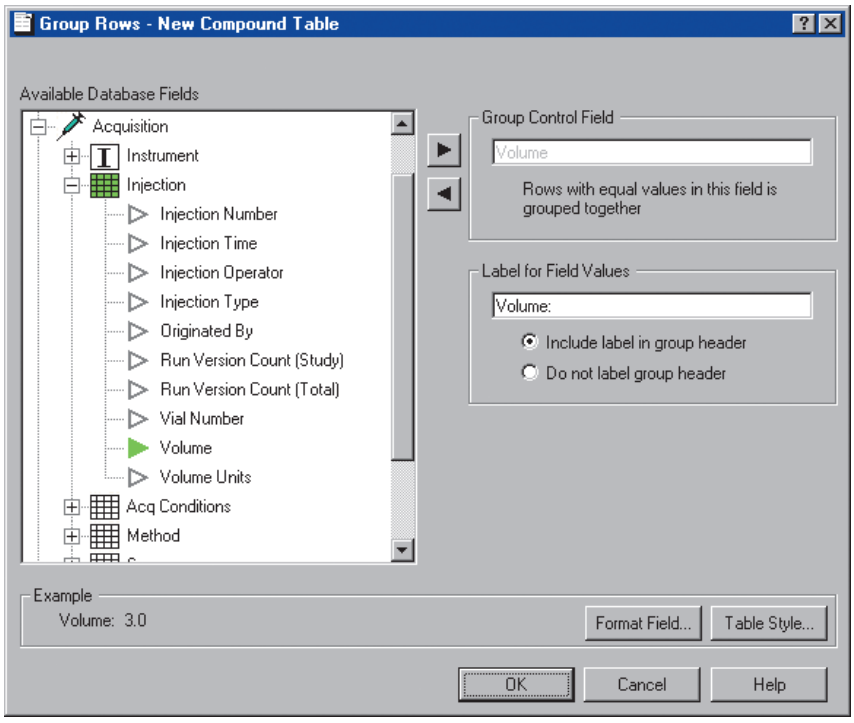



**Figure 20**
**Grouping criteria for statistical evaluation –in this case statistical evaluation should be done across those runs with the same injection volume**

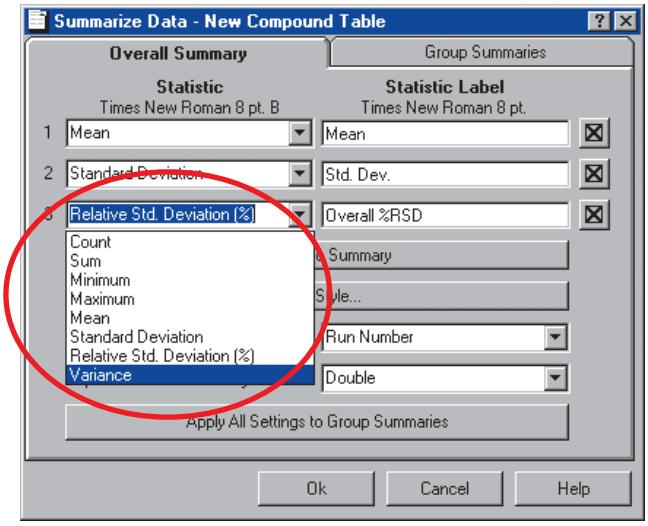



**Figure 21**
**Selecting statistical calculation procedures, showing the available calculation procedures**

After highlighting the name of the report template, see figure 18 where the template name is the first item in the list on the left, another selection tool can be used to select only specific compounds for reporting, see figure 22. This is then valid for the complete report template. The appropriate tool is named *Compounds* and is at the bottom of the screen.

### Including information from the Agilent 1100 Series well-plate sampler in the database

During setup of a sequence table using the Agilent 1100 Series well-plate sampler, entries for the *Plate id* can be used to characterize the used well-plates. These names or comments are accessible through ChemStore reports. Figure 23 shows how this information can be selected in a compound table for printing. Well-plate position, identification and type are entered in the custom field section.

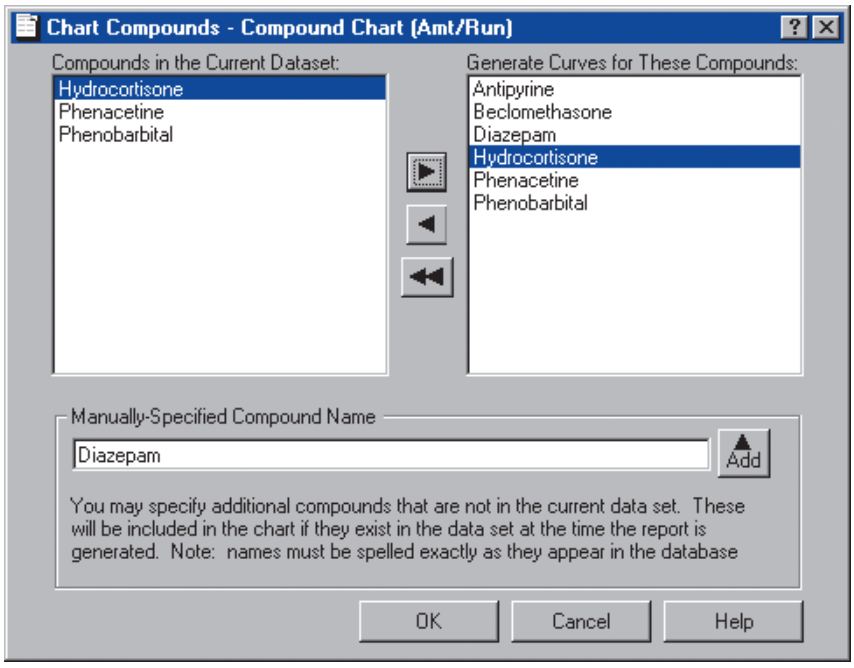



**Figure 22**
**Restriction of complete report template on specific compounds, showing how the selection of compounds for reporting can be done for the complete report template using the selected tool**

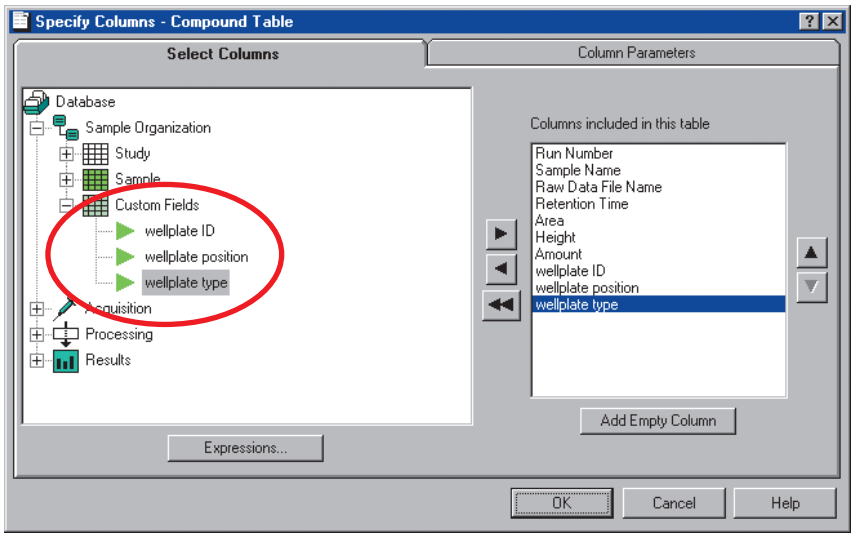



**Figure 23**
**Selecting well plate sampler parameters for printing using the pre-defined custom fields that are available for the Agilent 1100 Series well-plate sampler**

**Library test report**

| Run No. | Compound | RT | Amount | Well-Plate ID | Well-Plate Location | Well-Plate Type |
|---|---|---|---|---|---|---|
| 1 | Beclomethasone | 3.075 | 10.00 | t405 | D-12 | *96Agilent* |
| 1 | Hydrocortisone | 2.145 | 10.00 | t405 | D-12 | *96Agilent* |
| 1 | Hydrocortisone -acetate | 3.550 | 10.00 | t405 | D-12 | *96Agilent* |
| 2 | Phenobarbital | 2.230 | 10.00 | t405 | A-08 | *96Agilent* |
| 3 | Diazepam | 4.291 | 10.00 | p002 | A-09 | *384Agilent* |
| 4 | Phenacetin | 2.357 | 100.00 | p002 | A-11 | *384Agilent* |
| 5 | Antipyrine | 1.642 | 100.00 | p002 | B-03 | *384Agilent* |
| 6 | Doxycycline | 1.658 | 50.00 | p002 | C-03 | *384Agilent* |

**Figure 24**
**ChemStore report containing columns with Agilent 1100 Series well-plate sampler information**

In figure 24 an example of a compound table is shown, which – besides run number, name of the compound, retention time and amount – also contains information about the well-plate location, identification and type.

These well-plate identification and characterization tools can help to keep track of compound libraries relating to possible decomposition over time or similar purposes.

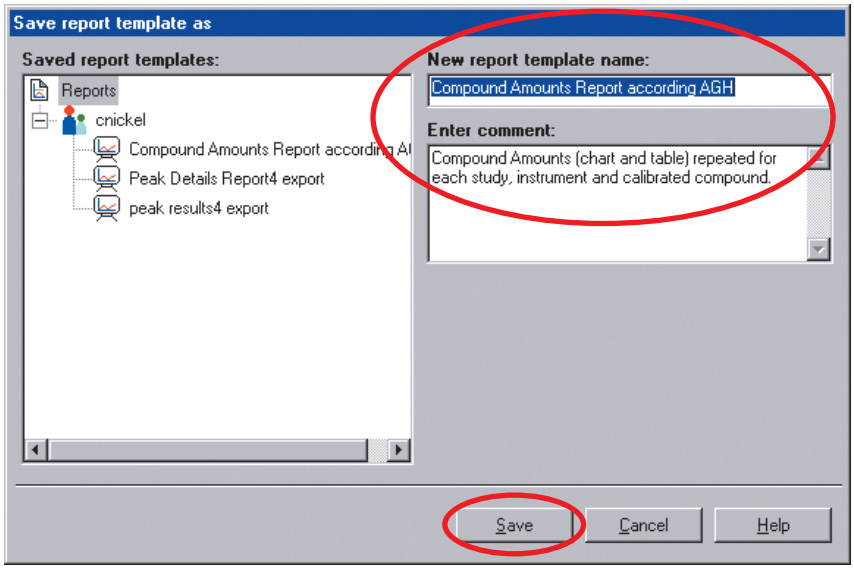



**Figure 25**
**Saving report templates – This routine also allows modifying a built-in report template and saving the modified template as new report template**

## Managing report templates

### Saving report templates

Report templates can be saved at any stage during report configuration, if the user has the right to *Create/Edit report templates*. To save the report template, click *Save* and type a unique name in the field *New report template name*, see figure 25. The left side displays all report templates that were created by the current user.

### Assigning report templates

Report templates are very important in the daily laboratories' work because they present the analysis result to supervisors, customers or auditors. The template development work is fairly intense because the report design requirements are quite often very complicated and detailed based on pharmacopoeia descriptions or other regulatory guidelines. It is therefore important to avoid unauthorized access or modifications to the report templates. But it also is important that all system users can use the report templates to print their final analysis report. This requires restricting access to report modifications (by granting or denying the user privilege *Create/Edit report templates*) but giving access to a broader group of instrument users to report printing.

ChemStore addresses this requirement by assigning report templates to dedicated users. This configuration enables to select and print reports based on custom report templates by denying access to report template modifications. The assignment of report templates to certain users also allows following the users work practices. For example, if user group A is working on stability studies, their lab manager will assign them access to their stability reports with trend charts but deny access to the routine quality control reports of user group B, who use the same instruments as user group A.

For example, to assign the recently created report template *Compound Amounts Report user1* to the built-in user named *operator*:

1 Choose *Assign to Users* under ChemStore's *Administration/ Settings*.
2 Select the *Report Template* tab, see figure 26.
3 Select *Operator* from the user drop-down list, see figure 27.
4 Select the report template *Compound Reports…* and click the right arrow in the middle of the menu, see figure 26.
5 Close the menu and log on as user *operator* (*Administration/ Change User*) with the password *operator*. Click the report template icon and make sure that the list includes the *Compound Amounts Report user1* as shown in figure 28.

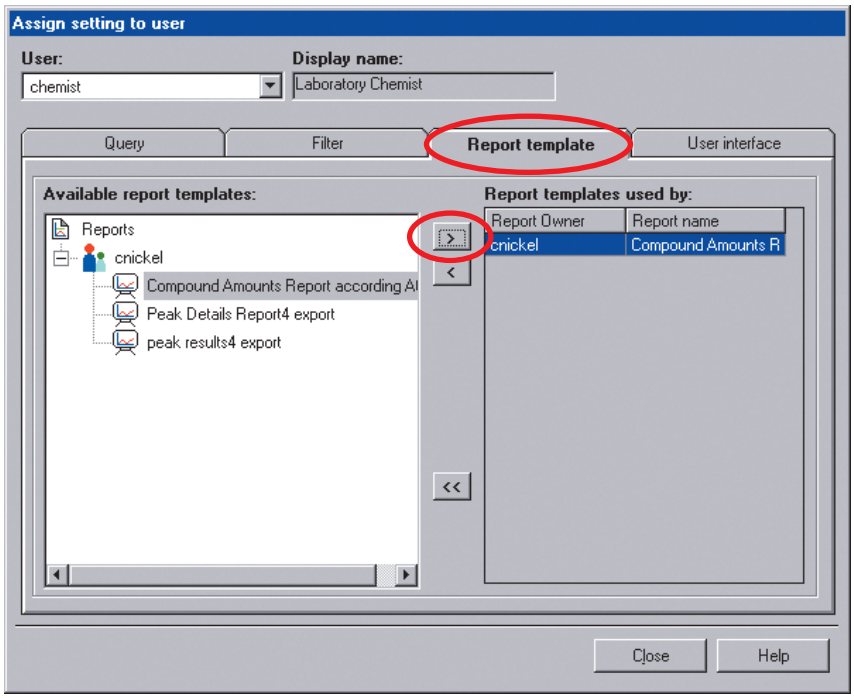



**Figure 26**
**Assigning report templates to users**

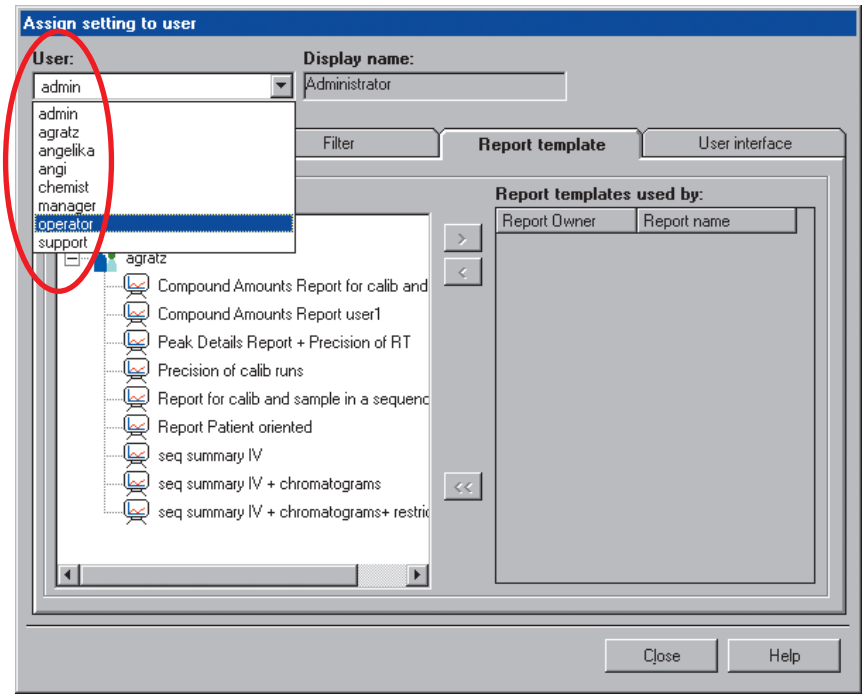



**Figure 27**
**Assigning report template to user operator**

## Printing reports

Reports can be displayed on the screen (*Print Preview*), printed on the printer, or saved to a file for easy data export. The report destination – *Screen*, *Printer*, *File* – is selected with the reporting smart icons or set in the report

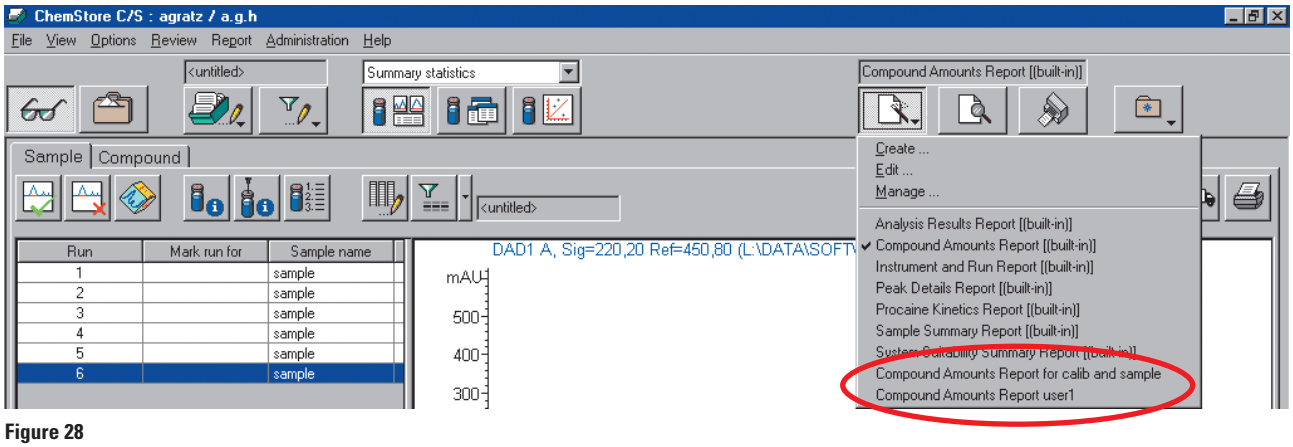



**Figure 28**
**Check that user operator has access to the custom compound amounts report**

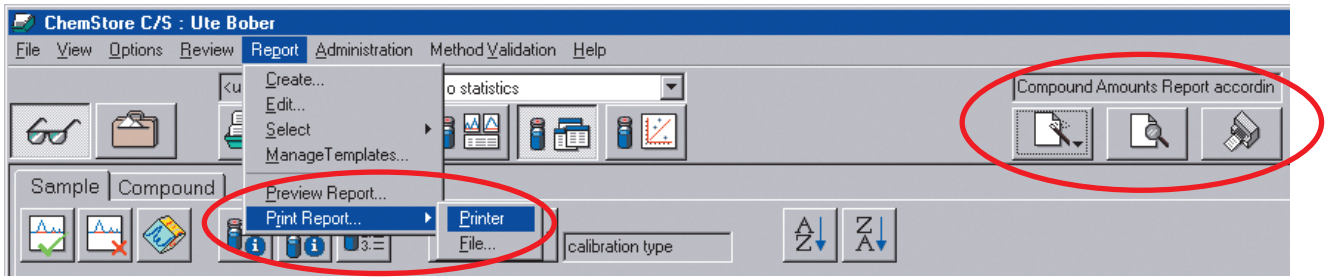



**Figure 29**
**Report printout options, showing the drop-down list, print preview and print icons (far right)**

menu as shown in figure 29. Available file formats are .CSV, .HTML or .XML. To print a report, do the following:

1 Select the data you want to use as described in section "Selection of data files for reporting – querying the database".
2 Select the report template from the drop-down list
3 Select the print destination.

Note that ChemStore reports can also print automatically at the end of a ChemStation sequence as described in section "Setting up ChemStore". This report allows for direct file export and printout but it does not offer print preview.

## Conclusion

ChemStation Plus opens up a new dimension of reporting possibilities. Although perfectly adequate for certain requirements, reporting with the ChemStation base software is limited to chromatographic data and associated results (such as plate number and resolution of peaks in a chromatogram) for predefined sequence-based sample sets. Reporting with ChemStation Plus, also referred to as ChemStore database reporting, offers in addition non-chromatographic sample data in custom fields (such as batch number and sample source information) and result meta data (such as approval and archive status with audit-trail information). It also enhances ChemStation base software reporting with query-based, cross-sequence, cross-instrument, cross-operator sample selection for reports.

ChemStore database reporting is a powerful tool for customized report configuration and supplements the easy and quick reporting possibilities of ChemStation base software. It allows the user to combine information across sequences and instrumentation in a single report. ChemStore reporting is designed to create the final analytical result as a paper copy. This result includes meta results such as trend charts and statistical summaries as well as all raw and meta data that might be required in an audit situation. This functionality helps users to get results faster without sacrificing compliance or completeness.

## References

1.
"Using Agilent ChemStation to generate summary reports for a single analysis or a sequence of analyses", *Agilent Technologies Application Note*, Publication Number 5988-9011EN

## Appendix

**Sequence Summary report on ChemStation Plus**

# Sequence Summary Report for CHEMST5.S


Report Last 15-Nov-01 9:48 Current Operator agratz

### Data Selection Criteria

**Query**

| | |
|---|---|
| Name: | <untitled> (agratz) |
| Run Selection: | Only latest runs |
| Conditions: | Raw Data.Data File IN ('NEW00052.D', 'NEW00053.D', 'NEW00054.D', 'NEW00055.D', 'NEW00056.D', 'NEW00057.D') |

**Standard Filter**

| | |
|---|---|
| Approval Status: | No Filter |
| Archive Status: | No Filter |
| Reprocessing Status: | All |

**User Filter**

| | |
|---|---|
| Condition: | None |

**Template**

| | |
|---|---|
| Compounds: | Only calibrated compounds |

### Overview

| Run No. | Vial | Inj No. | Audit | Sample | Sample Type |
|---|---|---|---|---|---|
| 1 | 2 | 1 | * | <unknown> | Calibration |
| 2 | 2 | 2 | * | <unknown> | Calibration |
| 3 | 2 | 3 | * | <unknown> | Calibration |
| 4 | 2 | 4 | * | <unknown> | Calibration |
| 5 | 2 | 5 | * | <unknown> | Calibration |
| 6 | 2 | 6 | * | <unknown> | Calibration |

Page 1 of 5

**Sequence Summary report on ChemStation Plus (continued)**

Sequence Summary Report — Report Printed 8-Feb-02 11:32

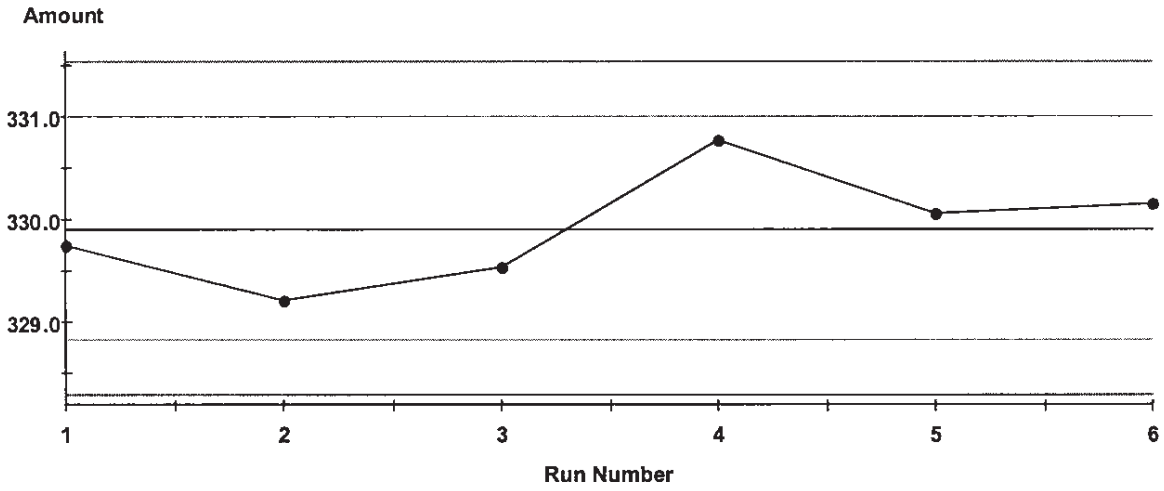
# Sequence Summary Report for CHEMST5.S

Study : chemstore test 2
Method: D:\HPCHEM\1\METHODS\ LINICHEM.M
Channel : DAD1 A, Sig=254,20 Ref=350,80
SampleType Calibration

Seq Modified : 15-Nov-01 10:45
Instrument : Instrument 1

Calib Level : 3

## Antipyrine




Peak Table

| Run No. | Data File | Audit | Peak Time | Resp. Factor | Area | Amount |
|---|---|---|---|---|---|---|
| 1 | NEW00052.D | * | 2.071 | 6.68650E-01 | 493.2 | 329.75 |
| 2 | NEW00053.D | * | 2.070 | 6.68814E-01 | 492.2 | 329.21 |
| 3 | NEW00054.D | * | 2.070 | 6.68864E-01 | 492.7 | 329.52 |
| 4 | NEW00055.D | * | 2.070 | 6.68673E-01 | 494.7 | 330.76 |
| 5 | NEW00056.D | * | 2.071 | 6.68716E-01 | 493.6 | 330.05 |
| 6 | NEW00057.D | * | 2.069 | 6.68691E-01 | 493.7 | 330.15 |
| Overall Mean | | | 2.070 | 6.68735E-01 | 493.3 | 329.91 |
| Overall %RSD | | | 0.03 | 0.01 | 0.2 | 0.16 |

**Sequence Summary report on ChemStation Plus (continued)**



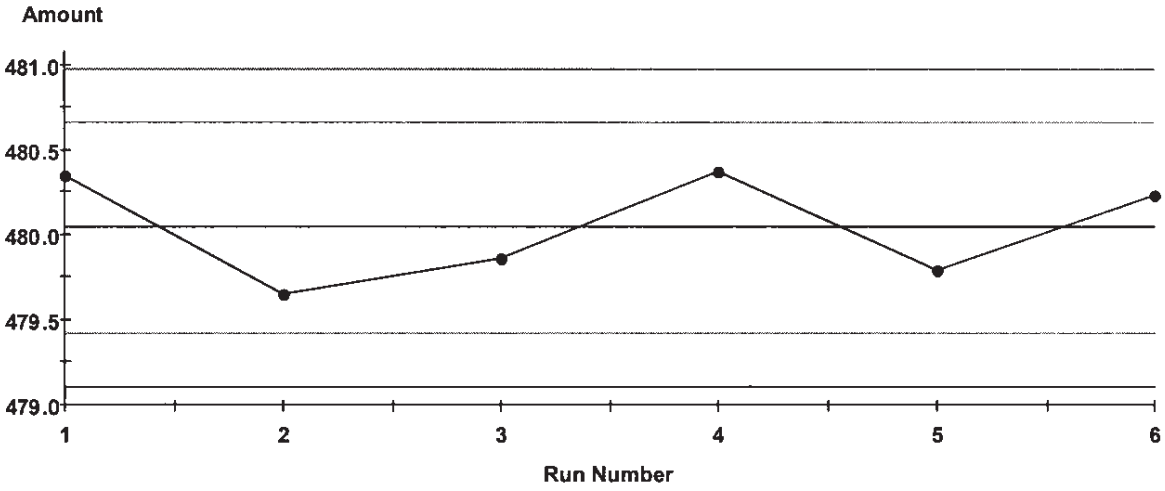
# Sequence Summary Report for CHEMST5.S

Study : chemstore test 2
Method: D:\HPCHEM\1\METHODS\ LINICHEM.M
Channel : DAD1 A, Sig=254,20 Ref=350,80
SampleType Calibration

Seq Modified : 15-Nov-01 10:45
Instrument : Instrument 1

Calib Level : 3

## Diazepam




Peak Table

| Run No. | Data File | Audit | Peak Time | Resp. Factor | Area | Amount |
|---|---|---|---|---|---|---|
| 1 | NEW00052.D | * | 5.084 | 9.87414E-01 | 486.5 | 480.35 |
| 2 | NEW00053.D | * | 5.085 | 9.87514E-01 | 485.7 | 479.65 |
| 3 | NEW00054.D | * | 5.085 | 9.87523E-01 | 485.9 | 479.86 |
| 4 | NEW00055.D | * | 5.085 | 9.87441E-01 | 486.5 | 480.37 |
| 5 | NEW00056.D | * | 5.085 | 9.87504E-01 | 485.9 | 479.78 |
| 6 | NEW00057.D | * | 5.084 | 9.87449E-01 | 486.3 | 480.23 |
| Overall Mean | | | 5.085 | 9.87474E-01 | 486.1 | 480.04 |
| Overall %RSD | | | 0.01 | 0.00 | 0.1 | 0.07 |

Sequence Summary Report

Report Printed 8-Feb-02 11:32

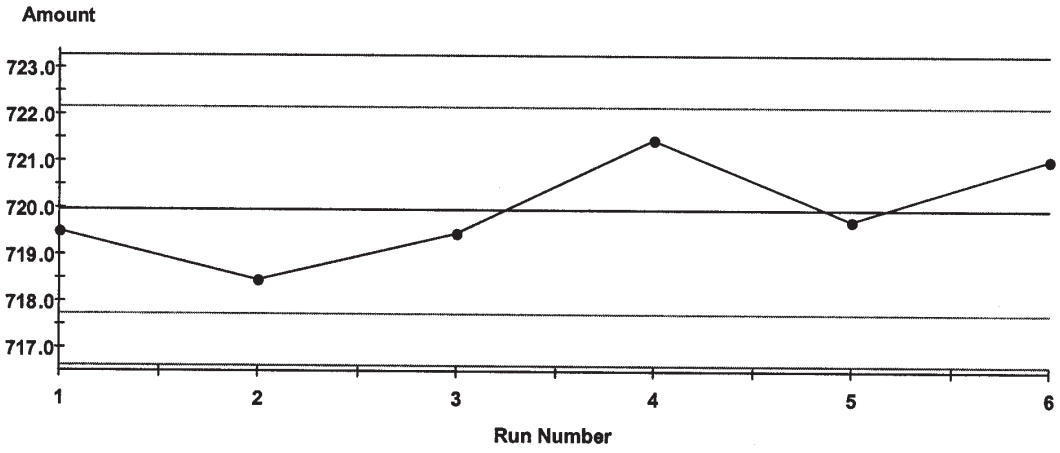
# Sequence Summary Report for CHEMST5.S

Study : chemstore test 2
Method: D:\HPCHEM\1\METHODS\ LINICHEM.M
Channel : DAD1 A, Sig=254,20 Ref=350,80
SampleType Calibration

Seq Modified : 15-Nov-01 10:45
Instrument : Instrument 1

Calib Level : 3

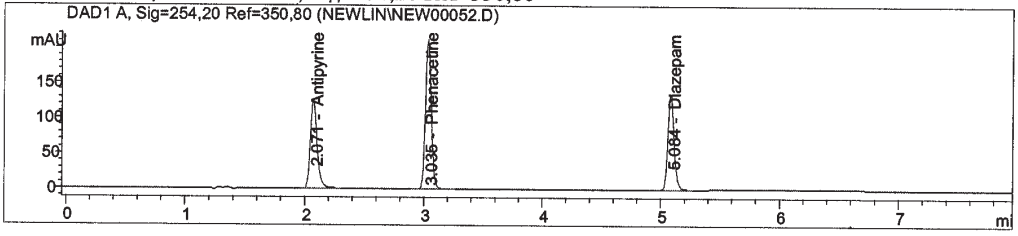
## Phenacetine




Peak Table

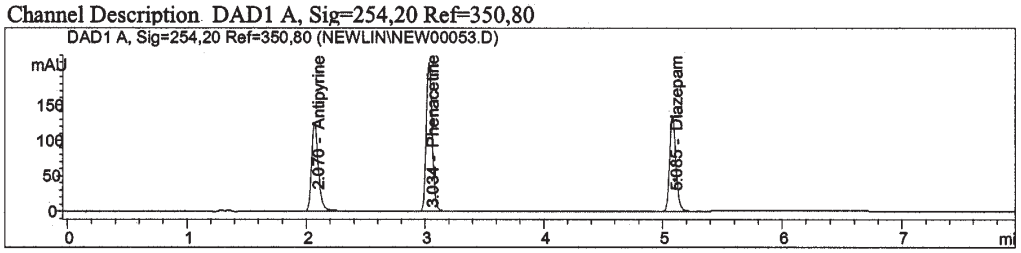
| Run No. | Data File | Audit | Peak Time | Resp. Factor | Area | Amount |
|---|---|---|---|---|---|---|
| 1 | NEW00052.D | * | 3.035 | 1.01010E+00 | 712.3 | 719.49 |
| 2 | NEW00053.D | * | 3.034 | 1.01032E+00 | 711.1 | 718.45 |
| 3 | NEW00054.D | * | 3.035 | 1.01033E+00 | 712.1 | 719.47 |
| 4 | NEW00055.D | * | 3.034 | 1.01011E+00 | 714.2 | 721.44 |
| 5 | NEW00056.D | * | 3.035 | 1.01021E+00 | 712.5 | 719.73 |
| 6 | NEW00057.D | * | 3.034 | 1.01006E+00 | 713.9 | 721.05 |
| Overall Mean | | | 3.035 | 1.01019E+00 | 712.7 | 719.94 |
| Overall %RSD | | | 0.02 | 0.01 | 0.2 | 0.15 |

Raw Data File Name NEW00052.D
Channel Description DAD1 A, Sig=254,20 Ref=350,80

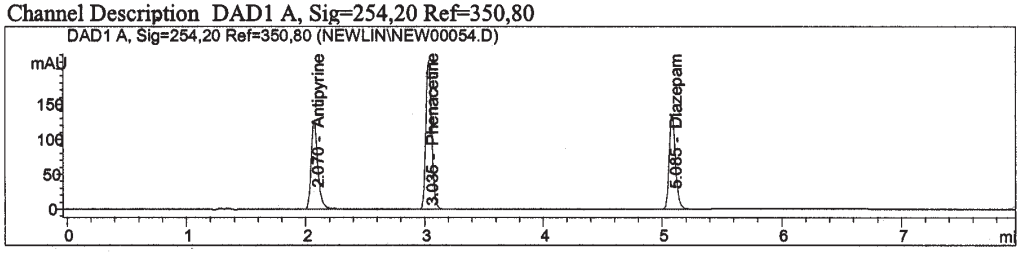


**Sequence Summary report on ChemStation Plus (continued)**

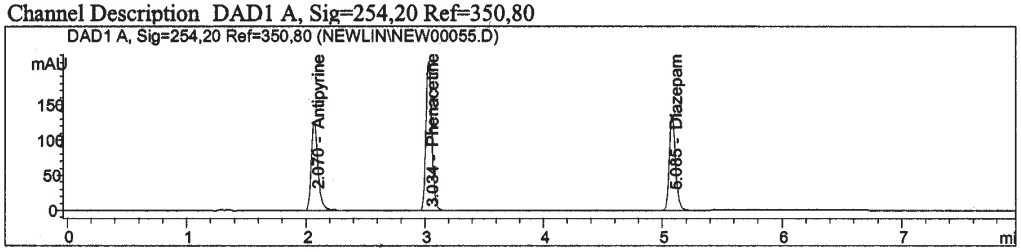
Raw Data File Name NEW00053.D
Channel Description DAD1 A, Sig=254,20 Ref=350,80



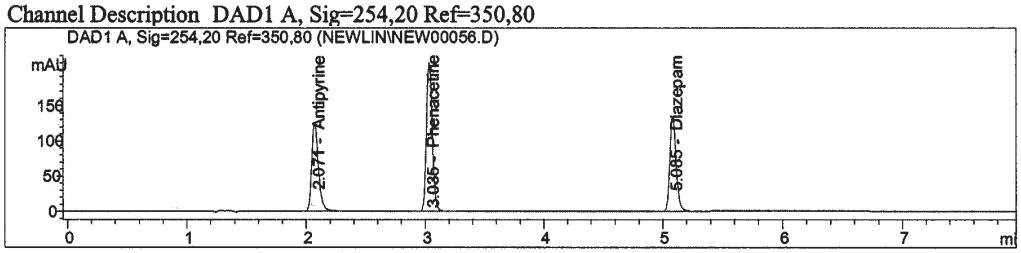

Raw Data File Name NEW00054.D
Channel Description DAD1 A, Sig=254,20 Ref=350,80



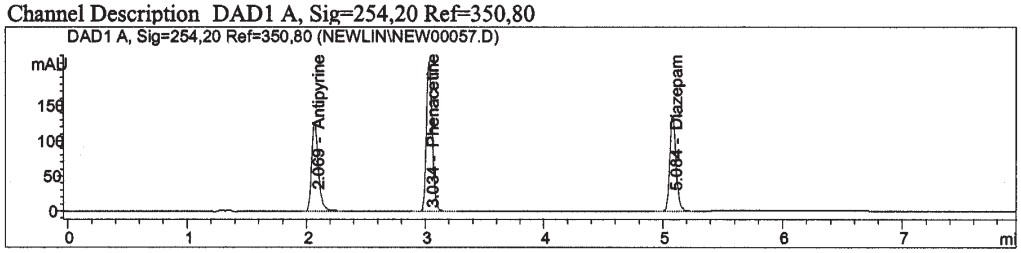

Raw Data File Name NEW00055.D
Channel Description DAD1 A, Sig=254,20 Ref=350,80




Raw Data File Name NEW00056.D
Channel Description DAD1 A, Sig=254,20 Ref=350,80




Raw Data File Name NEW00057.D
Channel Description DAD1 A, Sig=254,20 Ref=350,80



# System Suitability Summary Report


Report Last Modified: 20-Jan-00 13:08 Current Operator agratz

## Data Selection Criteria

**Query**

| | |
|---|---|
| Name: | <untitled> (agratz) |
| Run Selection: | Only latest runs |
| Conditions: | Raw Data.Data File IN ('CON00015.D', 'CON00016.D', 'CON00017.D', 'CON00018.D', 'CON00019.D') AND Method.Meth Saved EQUALS #2/14/02 8:35:51 AM# |

**Standard Filter**

| | |
|---|---|
| Approval Status: | No Filter |
| Archive Status: | No Filter |
| Reprocessing Status: | All |

**User Filter**

| | |
|---|---|
| Condition: | None |

**Template**

| | |
|---|---|
| Compounds: | Only calibrated compounds |

# System Suitability Summary Report

Study Name: **Systsuitability** Sample Name: **calanti+**
Instrument Name: **Instrument 1**
Method: **D:\HPCHEM\1\METHODS\ SYSSUIP.M**

Compound Name: **Diazepam**

## Peak Table

| Data File | Audit | Peak Time | Tail Factor | Theo.Plates | Resolution | Resp. Factor |
|---|---|---|---|---|---|---|
| ***Vial Number:*** | ***21*** | | | | | |
| CON00019.D | * | 5.983 | 1.11 | 2727.03 | 8.33 | 2.21489E-01 |
| CON00018.D | * | 5.984 | 1.10 | 2695.56 | 8.71 | 2.21489E-01 |
| CON00017.D | * | 5.990 | 1.10 | 2725.55 | 8.78 | 2.21489E-01 |
| CON00016.D | * | 5.986 | 1.11 | 2720.88 | 8.89 | 2.21489E-01 |
| CON00015.D | * | 5.998 | 1.10 | 2721.62 | 8.66 | 2.21489E-01 |
| **Mean** | | 5.988 | 1.11 | 2718.13 | 8.68 | 2.21489E-01 |
| **Std. Dev.** | | 0.0060 | 0.002 | 12.877 | 0.212 | 0.00000E+00 |
| **RSD** | | 0.10 | 0.22 | 0.47 | 2.45 | 0.00 |
| **Overall Mean** | | 5.988 | 1.11 | 2718.13 | 8.68 | 2.21489E-01 |
| **Overall Std. Dev.** | | 0.0060 | 0.002 | 12.877 | 0.212 | 0.00000E+00 |
| **Overall Variance** | | 0.00004 | 0.0000 | 165.8136 | 0.0450 | 0.00000E+00 |
| **Overall %RSD** | | 0.10 | 0.22 | 0.47 | 2.45 | 0.00 |

# Sample Summary Report

Agilent Technologies

Report Last Modified: 20-Jan-00 13:08 Current Operator agratz

**Data Selection Criteria**

**Query**

| | |
|---|---|
| Name: | <untitled> (agratz) |
| Run Selection: | Only latest runs |
| Conditions: | Sample Processing Parameters.Sample Type IN (´Calibration´, ´Sample´, ´Seq) |

**Standard Filter**

| | |
|---|---|
| Approval Status: | No Filter |
| Archive Status: | No Filter |
| Reprocessing Status: | All |

**User Filter**

| | |
|---|---|
| Condition: | None |

**Template**

| | |
|---|---|
| Compounds: | Only calibrated compounds |

**Sample Summary Report (continued)**

# Sample Summary Report

Study Name: **Systsuitability** Instrument Name: **Instrument 1**

DA-Method: **SYSSUIP.M**

**Sample Run Table**

| Sample Name | Injection Time | Data File | Smp.Type | Smp. Amount |
|---|---|---|---|---|
| Data Path: L:\DATA\SYSSUI\ | | | | |
| calanti+ | 11-Feb-02 8:30 | CON00001.D | Calibration | 0.00 |
| calanti+ | 11-Feb-02 8:39 | CON00002.D | Calibration | 0.00 |
| calanti+ | 11-Feb-02 8:48 | CON00003.D | Calibration | 0.00 |
| calanti+ | 11-Feb-02 8:57 | CON00004.D | Calibration | 0.00 |
| calanti+ | 11-Feb-02 9:06 | CON00005.D | Calibration | 0.00 |
| urine mueller | 11-Feb-02 9:15 | CON00006.D | Sample | 0.00 |
| urine mueller | 11-Feb-02 9:24 | CON00007.D | Sample | 0.00 |
| urine mueller | 11-Feb-02 9:33 | CON00008.D | Sample | 0.00 |
| antiprrine+ | 11-Feb-02 9:51 | CON00010.D | Seq Control | 0.00 |
| antiprrine+ | 11-Feb-02 10:01 | CON00011.D | Seq Control | 0.00 |
| urine Kaiser | 11-Feb-02 10:10 | CON00012.D | Sample | 0.00 |
| urine Kaiser | 11-Feb-02 10:19 | CON00013.D | Sample | 0.00 |
| urine Kaiser | 11-Feb-02 10:28 | CON00014.D | Sample | 0.00 |
| calanti+ | 11-Feb-02 10:37 | CON00015.D | Calibration | 0.00 |
| calanti+ | 11-Feb-02 10:46 | CON00016.D | Calibration | 0.00 |
| calanti+ | 11-Feb-02 10:55 | CON00017.D | Calibration | 0.00 |
| calanti+ | 11-Feb-02 11:04 | CON00018.D | Calibration | 0.00 |
| calanti+ | 11-Feb-02 11:13 | CON00019.D | Calibration | 0.00 |
| urine Kline | 11-Feb-02 11:22 | CON00020.D | Sample | 0.00 |
| urine Kline | 11-Feb-02 11:31 | CON00021.D | Sample | 0.00 |
| antipyrine+ | 11-Feb-02 11:40 | CON00022.D | Seq Control | 0.00 |
| antipyrine+ | 11-Feb-02 11:49 | CON00023.D | Seq Control | 0.00 |
| antipyrine+ | 11-Feb-02 11:58 | CON00024.D | Seq Control | 0.00 |

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**www.agilent.com/chem/nds**



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