

Agilent ChemStore C/S

ChemStore Admin Tools User Guide

Notices

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This handbook is for a module of the Agilent ChemStation Plus software. In the section “Introduction” on page 4 you will find details about the module and the revision of the module that this book is intended to be used for.

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A **WARNING** notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a **WARNING** notice until the indicated conditions are fully understood and met.

Contents

1. Introduction.....	4
2. Installation and Configuration	5
Prerequisites	5
Installation Procedure	5
Initial start-up and configuration	7
3. Operation	8
DB Health Monitor	8
Process Monitor	12
Expert user mode.....	14

1. Introduction

The ChemStore Admin Tools are an addition to the ChemStore Admin Client offering ChemStore administrators additional tools to check the filling level and health of a ChemStore database as well as a monitoring tool for archive/delete processes performed on a ChemStore server database.

It is a plain monitoring, analyzing and reporting tool with no data interaction capabilities. The usage is restricted to ChemStore administrators only. The Tools consist of three independent components: The DB Health Monitor for generation of a database overview report, the Process Monitor which allows on-line monitoring of time consuming archive and delete processes and the password protected Expert Users Mode which is restricted to trained Agilent technicians for in depth troubleshooting of fatal errors in case of a database corruption caused e.g. by a server outage or an incomplete Oracle roll-back.

Unlike the Web-based ChemStore Admin Client the Admin Tools are installed on selected clients only but support multiple ChemStore and Oracle revisions. The descriptions in this document refer to revision 1.0.8 of the Admin Tool program. The revision information can be displayed in the menu **Help > About**.

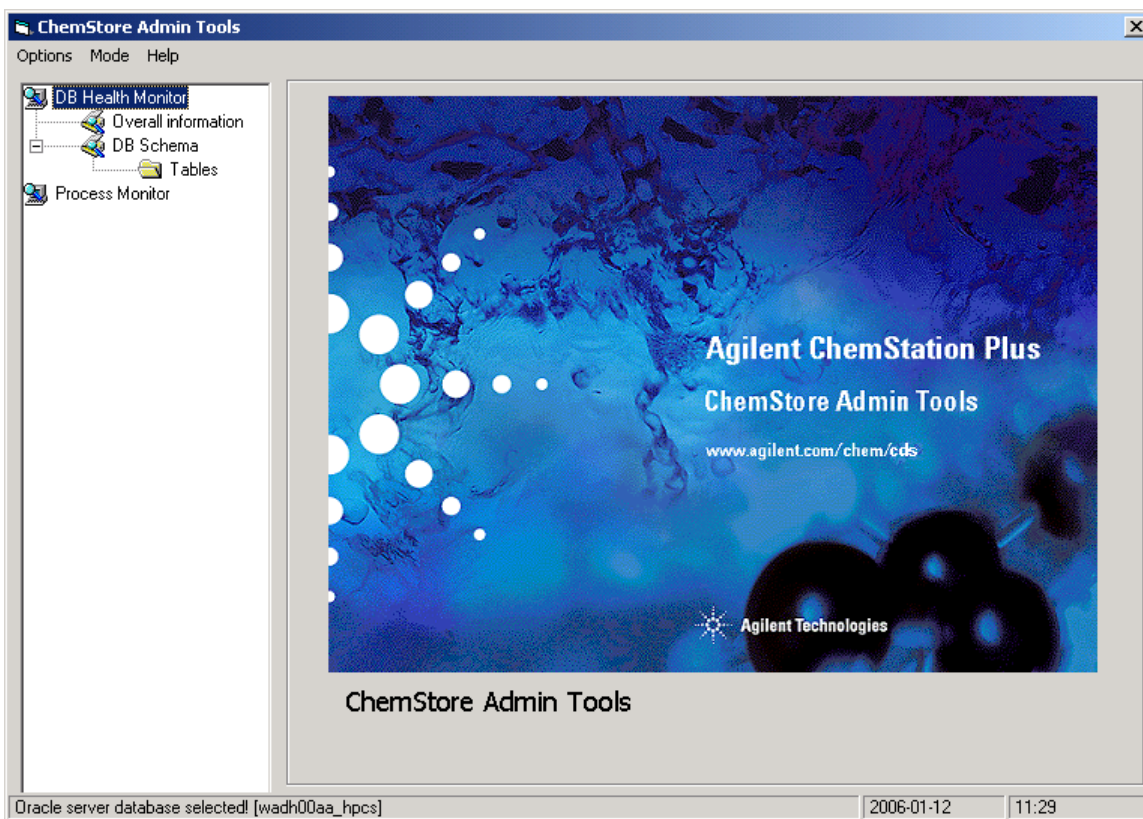


Figure 1 ChemStore Admin Tools main navigation screen

2. Installation and Configuration

Prerequisites

The A.1.0.8 version of ChemStore Admin Tools is supported on Windows XP® operating systems only. It got tested and qualified with Service Release 2 for Windows XP. The supported Oracle® version is Oracle 10.2.0.3.0. Further on it requires the Oracle Provider for OLE DB 10.2.0.3.0. The program needs to be installed on a ChemStore stand-alone or client system.

The ChemStore Admin Tools are initially supported with ChemStore stand-alone or client and server revisions B.04.01. Test results and compatibility with earlier versions will be announced on the update web-page mentioned in next section.

The Adobe® Acrobat Reader® 8.0 or higher needs to be installed to display the user manual.

The installation requires less than 5 MB hard-disk space and no other hardware requirements as specified for the basic ChemStation Plus system.

Updates

New versions of the Admin Tools are released independently from the base product. You can get the latest information and version of the tools on

www.chem.agilent.com/en-US/Support/Downloads/Patches/ChemStore/Pages/ChemStore_Admin.aspx

Installation Procedure

Perform the following steps to install the ChemStore Admin Tools software on a ChemStore client system.

- 1** Log-on to Windows as a user with administrative capabilities.
- 2** Put the ChemStation Plus Client installation CD into the CD-ROM drive or open the downloaded installation file container and browse to \support\tools\Admin Tools\ and double-click the file adminTools_ver108_setup.exe. The ChemStore Admin Tools set-up program will start and will lead you through a number of installation screens.
- 3** Enter the path to install the ChemStore Admin Tools software. By default the software is installed in a subdirectory under the ChemStore directory (\chem32\chemstor). This is the recommended path.
- 4** Click the button **Next**.
- 5** In the **Select Components** dialog keep all items selected and click the button **Next**.

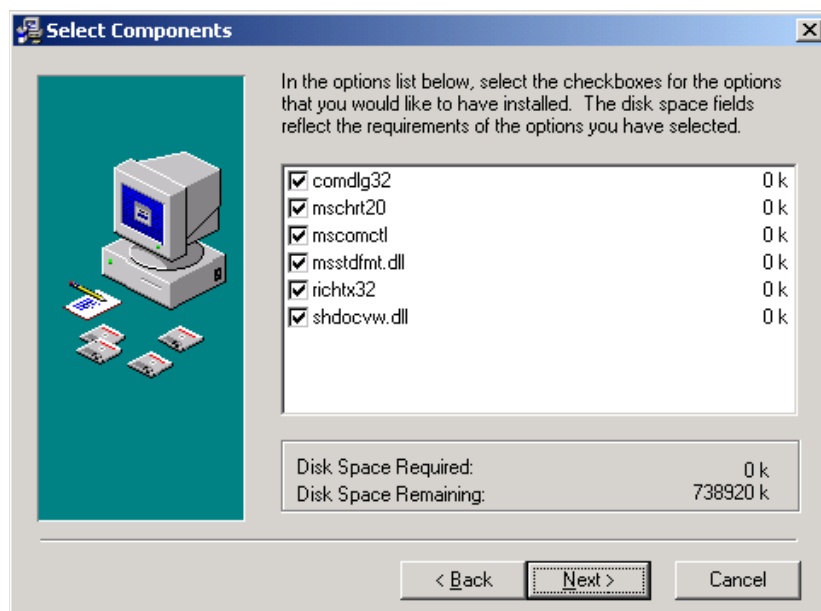


Figure 2 ChemStore Admin Tools Installation Components

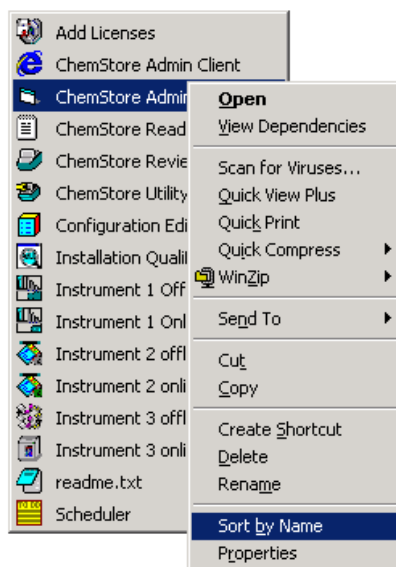
6 Select a Program Manager Group to specify a location for the start-up icon in the Windows Programs group. The default value is **Agilent ChemStation**.

7 Click the button **Next** and the installation process starts.

9 When you see the confirmation screen, click the button **Finish** to exit the installation.

10 Reboot the PC when prompted.

11 Resort the ChemStation Plus icons for your convenience.



Initial start-up and configuration

Before the initial start up of the ChemStore Admin Tools it is recommended to launch the ChemStore Review client and verify a working client/server connection. To start the Admin Tools:

- 1 Start the ChemStore Admin Tools by selecting **Programs > AgilentChemStation > ChemStore Admin Tools** from the Windows **Start** menu.
- 2 Click on the **Select Database** button in the login dialog to select a database. The database selection window will initially show no entries.

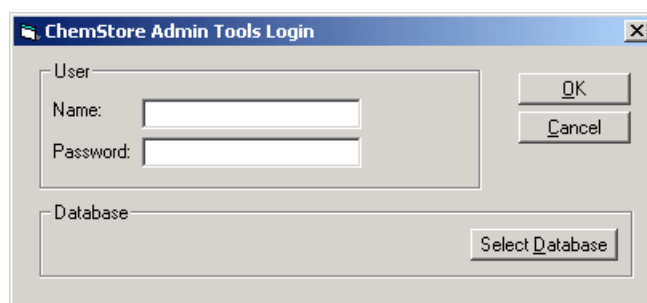


Figure 3 ChemStore Admin Tools Login

3 If you want to connect to a ChemStore server database check the 'Server TNS name' button and enter the SQL Net name of the database that consists of the server name and the database alias, e.g. *csserver_hpcs*.

If you want to connect to a ChemStore Stand-Alone database check the 'Standalone' button and press the **Browse** icon to select a standalone database. Press the **OK** button to activate this selection.

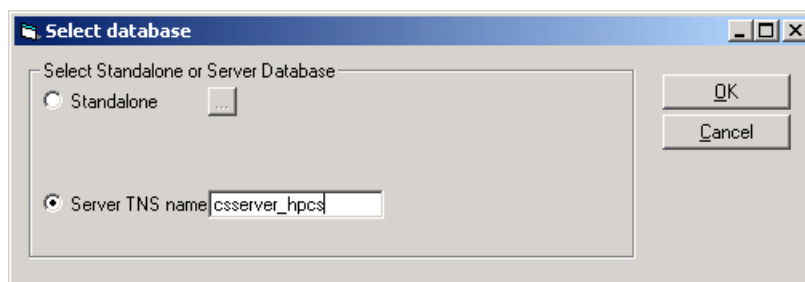


Figure 4 Select database dialog

4 Back to the login dialog enter the name and password of a ChemStore user with administrative privileges. Click the button **OK**.

3. Operation

DB Health Monitor

The DB Health Monitor allows ChemStore administrators to generate a database overview report as well as a detailed verification check of all ChemStore related database tables, table indices, and table field types.

To start an overall report, click the **overall information** branch under the DB Health Monitor tree. The report returns items like:

- Number of ChemStore specific database tables
- Estimated size of a database export file
- Number and names of studies, users, custom fields, report templates, and archive units
- Number of runs, raw data files, queries, number of archived runs
- name and sizes of all archive units

The outcome of the report can be saved to a text file by the menu **Options > Write results to file**.

Example: The following example report got generated on a 20 GB database. Certain numbers and names got changed to reduce the overall size of the report.

```
=====
OVERALL DETAILS for csserver_hpcs                               as of 16 Jan, 2006
=====

CS Version:                B.03.02
Build number:              65
Last table ID number:      10233214
                                     General revision
                                     information

Tables owned by
internal ChemStore User:    179
                                     ChemStore specific
                                     tables
Tables owned by
Method Validation Pack:    0
                                     MVP specific tables

Approx. db export size:     19,107.98 (Mb)
                                     Database export size
=====

Total number of studies:    8
                                     General study overview

ID      Study Name
-----
1002     Lab A
1003     LAB B
1201     Quality Control
1401     Method Develop.
1402     Lab C
1403     Lab D
1004     Lab E
1005     Lab F

=====

Total number of users:      17
                                     User list, separating
                                     active from non-active
                                     users
User ID #  User Logon Name  (active users)
-----
101        support
102        admin
103        manager
104        chemist
105        operator
```

```

1044      castills
5499      oqusercs
5543      oquser
49722     oqchemistcs
 53748    agilent
67039     Testuser
170980    Tuser1
230007    Tuser2
8485045   demo
  
```

```

User ID #  User Logon Name      (non-active users)
-----
  
```

```

100      (built-in)
2479     oquser1
15454    OQUSEROS
  
```

```

=====
Number of Runs:      203718
Raw Data Files:      203223
Injections:          306594
Chromatograms:       205528
Clients:             25
Instruments:         63
  
```

Database content for
estimating the filling
level

```

-----
Peaks:              853692
Compounds:          4733
  
```

```

-----
Audit Trail:        569758
Max rn_id Number:   10233189
  
```

```

-----
Chromatograms:      205528
Max rn_id:          10233189
Max cg_id:          10233190
Max so_id:          10233156
  
```

```

-----
Spectra:            348
Max rd_id:          10232869
Max sp_id:          10232890
Max so_id:          10232891
  
```

```

-----
Methods:            106162
Max mt_id:          10233189
  
```

```

-----
Sequences:          106163
Max sq_id:          10231405
  
```

```

-----
Stored Objects:     1714394
Max so_id:          10233213
  
```

```

-----
Method Objects:     895709
Max mt_id:          10233189
  
```

```

-----
Raw Data Objects:   1456848
Max rd_id:          10233189
  
```

Custom Field ID Custom Field Name

Number of Filters

Number of Filters: 14

=====

Total number of reports: 3

Report ID	Report Name
100	Analysis Results Report
198	Instrument and Run Report
256	Compound Amounts Report

Report templates

Sample Names

Stored Queries

Stored Queries: 73

Study Name	# Run in
09-10008015	1561
09-10008615	42715
09-10008616	1115
09-10010889	2885
09-10011010	1085
09-10011017	7456
09-10011022	49443
09-10011036	13464

Numbers of runs per
study

=====

ARCHIVE DETAILS

=====

Archived Raw Data: 365170
Archived Runs: 365410

Archive statistics

Total number of archive units:344

Total number of archive files: 9,808.35 (Mb)

Archive Unit	Archived Runs	Archived Size (Mb)	Last Changed
2612	4	0.12	2002-06-22 10:05:12
2614	177	2.66	2002-06-22 10:35:12
2615	22	0.62	2002-06-22 11:16:39
2616	16	0.69	2002-06-22 11:25:44
3219	2	0.13	2002-06-22 12:05:12

Archive sizes on disk

. . .

Number of Runs Archived: 386350
Never Archived: 194744
Archive Failed: 120
Archive Pending: 0
Archived But not Deleted: 1916
Archive Running: 0
Delete Failed: 0
Delete Pending: 0

De-archive status information:

```
Archive ID      = 1612
Archive TS     = 2002-02-21 15:49:08
Archive text   = Study Method Development Q1 2002
Archive file   = D:\DATA\archive\020120_01
Archive size   = 0.52 (in Mb)
Archived runs  = 14 (8 of them in database)
```

De-archiving level of
partially or never de-
archived units

```
Archive ID      = 2615
Archive TS     = 2002-08-22 11:49:39
Archive text   = Study Method Development 10 2002
Archive file   = D:\DATA\archive\020622
Archive size   = 0.62 (in Mb)
Archived runs  = 22 (0 of them in database)
```

Weekly monitoring of the estimated size of the database export file can be used to estimate the growth rate of the database or to control efficiency of the archive/delete operations. Once a database reaches its predicted maximum size the archive/delete process needs to be used to keep this size constant.

The numbers reported in the overall report are also important for the Agilent Support line to get a good estimation about the size and content of your database.

NOTE	Generating a database overview report includes execution of extensive SQL queries. This might temporarily reduce the database performance. The first overview report should be generated while the database is under weak load.
-------------	---

In contrast to the dynamic data presented in the overall report the **DB Schema / Tables** reports are rather static and don't need to be repeated on a frequent base. The check can be executed on all tables or on individual database tables. Click on the **DB schema > tables** branch of the tree view in order to select all tables or select one table out of the tables list. The context sensitive selection is displayed right to the **Start** button.

The report can be used to check for missing ChemStore specific database tables e.g. after a database migration or a database maintenance by using Oracle export/import. The table check is done versus revision specific reference files stored under c:\chem32\ChemStor\AdminTools\scripts.

In addition the tool checks the field types of each table column and compares it to the reference. The field types do not change unless the database gets manually altered.

NOTE	A detailed explanation of the ChemStore database tables and the relation between the tables can be found in the ChemStore database dictionary and data model documents. To get a copy of this database design documents contact your local Agilent support representative. A Confidential Disclosure Agreement needs to be signed to exchange this information.
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Oracle table indices are the third item to be checked with this type of report. Oracle database administrators might add or recreate indices for performance tuning and optimization purposes. However indices should not be deleted if they are part of the default index set provided with the installation. Unique indices guarantee the uniqueness of table data and removing this type of index can cause data corruption.

The DB tables report checks the presence of all default indices and additional ones.

Process Monitor

The Process Monitor is an administrative feature that allows on-line monitoring of time consuming archive and delete processes. The ChemStore Admin Client as installed as part of the ChemStore client is operated by the same server service as the Archive/Delete process and due to the heavy load on this service the Admin Client is not responsive during an archive/delete operation.

As these kinds of operations can last up to multiple hours, depending on the database and archive size, the ChemStore Admin Tool fills this gap.

Especially when establishing an archive/delete workflow on a database it is very important to run some benchmark tests on the performance. As archiving/deleting performs the best while the database is in idle mode, these maintenance operations are typically scheduled during the night. Performance measurements achieved by the Admin Tools allow an estimation of the data package size to be archived and deleted during one night.

The monitoring results are displayed in graphical as well as a tabular form. Tabular results can be written to a report by enabling the **Log monitor results** checkbox. These reports get stored under the temporary path specified under **Admin Tool Options**. The reports can be used for quantifying the archive/delete performance as part of the workflow planning.

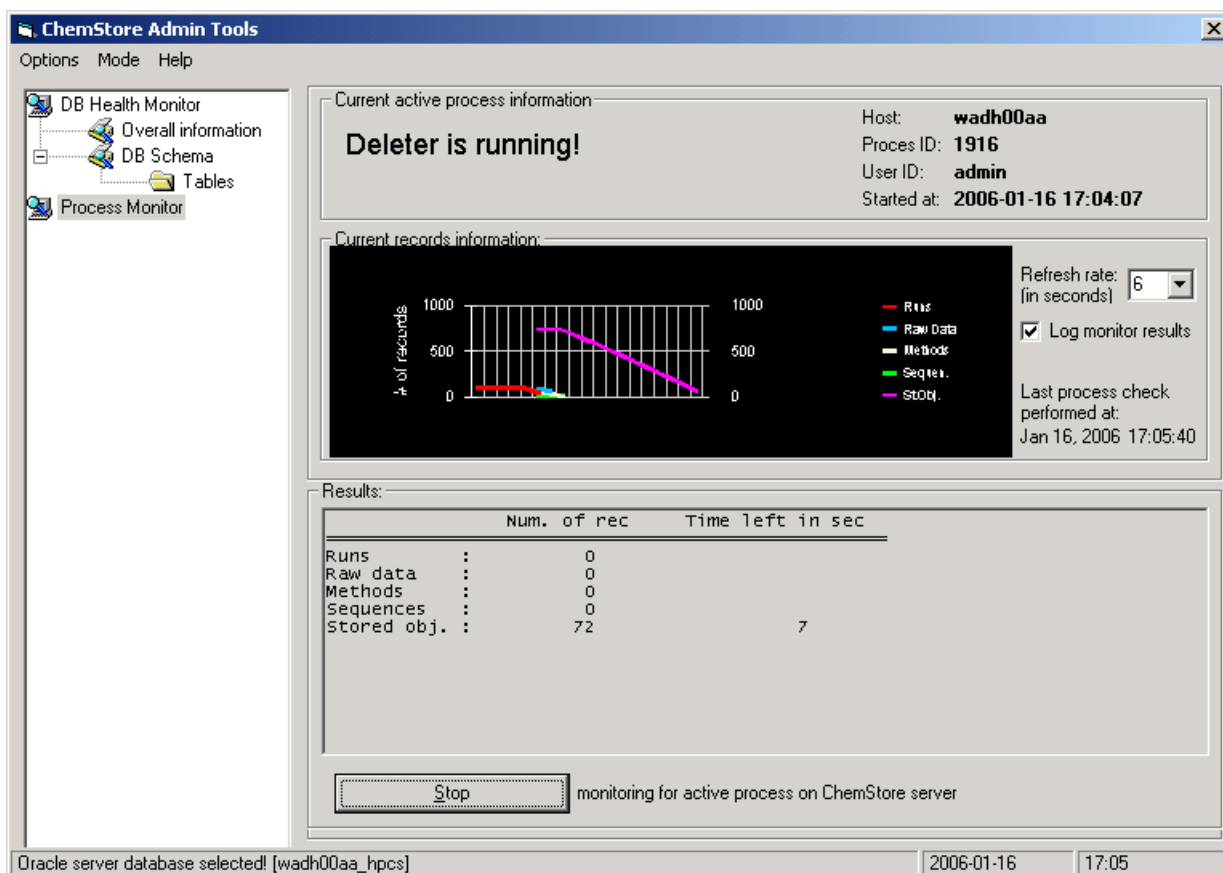


Figure 4 Archive/delete monitoring of 95 runs, Refresh rate 6 sec

Example: Archive/Delete operation of 95 runs, Refresh rate 6 sec

```

"[01-16-2006 17:03:27] [Archiver is running!]
Num. of rec      Time left in sec
=====
Runs      :      95      In progress...
Raw data   :      0
Methods    :      0
Sequences  :      0
Stored obj. :      0

"[01-16-2006 17:03:33] [Archiver is running!]
Num. of rec      Time left in sec
=====
Runs      :      95      In progress...
Raw data   :      0
Methods    :      0
Sequences  :      0
Stored obj. :      0

"[01-16-2006 17:04:04] [Archiver is running!]
Num. of rec      Time left in sec
=====
Runs      :      95      In progress...
Raw data   :      0
Methods    :      0
Sequences  :      0
Stored obj. :      0

"[01-16-2006 17:04:17] [Deleter is running!]
Num. of rec      Time left in sec
=====
Runs      :      54      In progress...
Raw data   :      95      In progress...
Methods    :      42      In progress...
Sequences  :      9       In progress...
Stored obj. :     737      In progress...

"[01-16-2006 17:04:33] [Deleter is running!]
Num. of rec      Time left in sec
=====
Runs      :      0
Raw data   :      0          Done
Methods    :      8          1
Sequences  :      9       In progress...
Stored obj. :     737      In progress...

"[01-16-2006 17:05:40] [Deleter is running!]
Num. of rec      Time left in sec
=====
Runs      :      0
Raw data   :      0
Methods    :      0
Sequences  :      0
Stored obj. :      72          7

"

"[01-16-2006 17:05:46] [Deleter is running!]
Num. of rec      Time left in sec
=====
Runs      :      0
Raw data   :      0
Methods    :      0
Sequences  :      0
Stored obj. :      6          1

```

Process started at 17:03

Archiving completed after 37s

Deleter started after XML file generation

Deleter finished after 89s

The graphical display allows a visual control of the delete process. ChemStore data consist of large binary data (stored objects) related to Raw Data, Methods and Sequences of a certain run. The delete process is not executed on a run by run base but object type based. The first objects to be deleted are the runs, followed by the associated raw data, methods, sequence, and finally the stored objects. Further details on the Archive/Delete process can be found in the **ChemStore Concepts Guide**.

Stored objects are the largest part of an archive unit and deletion of this data type is the most time consuming part. As the default report sampling interval is 2 sec it might not be suitable for slow processes that last several hours. The report **Refresh Rate** can be raised up to 300 sec.

Expert user mode

The password protected expert users mode is restricted to trained Agilent technicians for in depth troubleshooting of fatal errors in case of a database corruption caused e.g. by a server outage or an incomplete Oracle roll-back.

CAUTION

Generating expert user mode reports creates temporary database tables that can drop the database performance significantly. The report should be generated while the database is idle.
