SampleTrack^{TM}

SampleTrack Manual
User Guide

Version 002

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This manual was written by

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Special thanks to Birk Schütz who developed the Web interface.

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Rheinstetten, Germany

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Contents

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Warnings and Notes

2

Warnings and Notes

2.1

There are two types of information notices used in this manual. These notices highlight important information or warn the user of a potentially dangerous situation. The following notices will have the same level of importance throughout this manual.

Note: Indicates important information or helpful hints

⚠

WARNING: Indicates the possibility of severe personal injury, loss of life or equipment damage if the instructions are not followed.

Contact for Additional Technical Assistance

2.2

For further technical assistance please do not hesitate to contact your nearest BRUKER dealer or contact us directly at:

BRUKER BioSpin GMBH
am Silberstreifen
D-76287 Rheinstetten
Germany

Phone: + 49 721 5161 0
FAX: + 49 721 5171 01
Email: sampletrack@bruker-biospin.de
Internet: www.sampletrack.de
or www.bruker-biospin.de

Introduction to Bruker LIMS

3

Laboratory Data Management Today

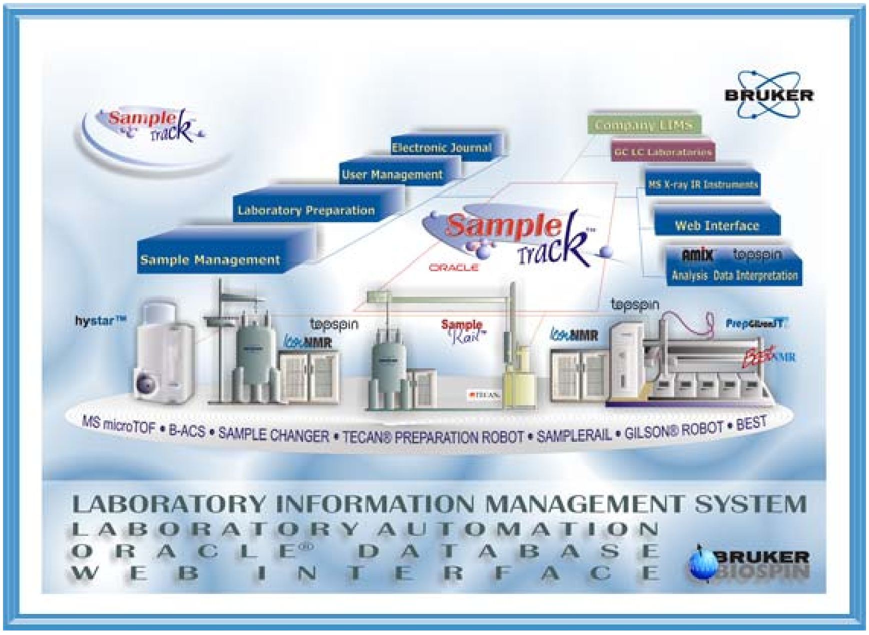
3.1

The steadily increasing number of samples in analytical spectroscopy means that laboratories have to deal with a massive data throughput. This is created on the one side by spectral data and analytical reports and on the other side by data archival, referencing and distribution. This situation, along with GLP requirements, FDA regulations, and ISO 9000 certification, means that the instrumentation in analytical laboratories have to be linked to an existing corporate LIMS. Increasingly, many chemical, pharmaceutical and biotech companies not only have their QA/QC processes integrated via LIMS, but also their R & D departments, where typically BRUKER NMR, FT-IR, and mass spectrometers are to be found. Therefore, many industrial users are now seeking to obtain a LIMS connection for BRUKER spectrometers. Traditional LIMS programs are laid out more for chromatography and for the very widespread, less costly analytical instrumentation. They do not usually include NMR spectroscopy. SampleTrack™ has been designed to fill this gap!

See also: SampleTrack Planning Questionnaire (http://www.bruker-biospin.de/NMR/automat/samtrac/samtrac6.html)

or the *SampleTrack™ homepage ((http://www.sampletrack.de/)*

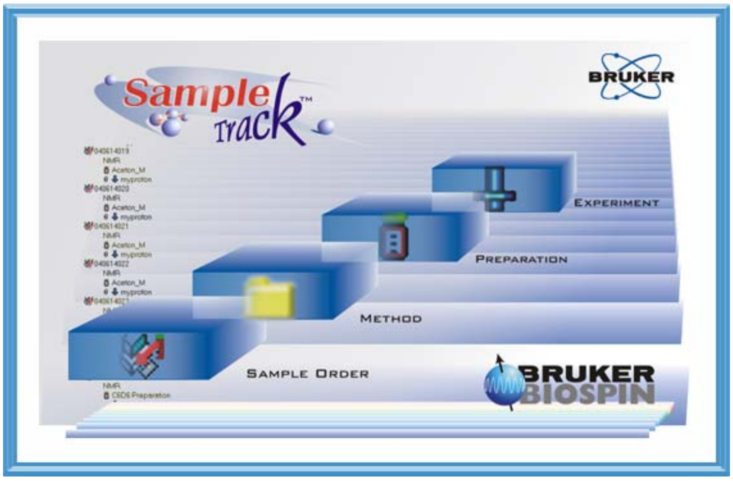
Figure 3.1. Laboratory Data Management - LIMS



Bruker Laboratory Information and Management System 3.2

SampleTrack™ is a Laboratory Information and Management System with a standardized interface for BRUKER spectrometers. It is a software package that provides the link between the analytical laboratory, the synthesis laboratory and the information processing department. More importantly, it is a software tool for the laboratory network that coordinates all automation steps in analytical measurements. It monitors the activity on the laboratory floor, and provides chronological precise and detailed information on each step along a sample's path. SampleTrack™ provides complete sample tracking for the NMR laboratory within a modern research environment.

Figure 3.2. SampleTrack™ - Worksteps



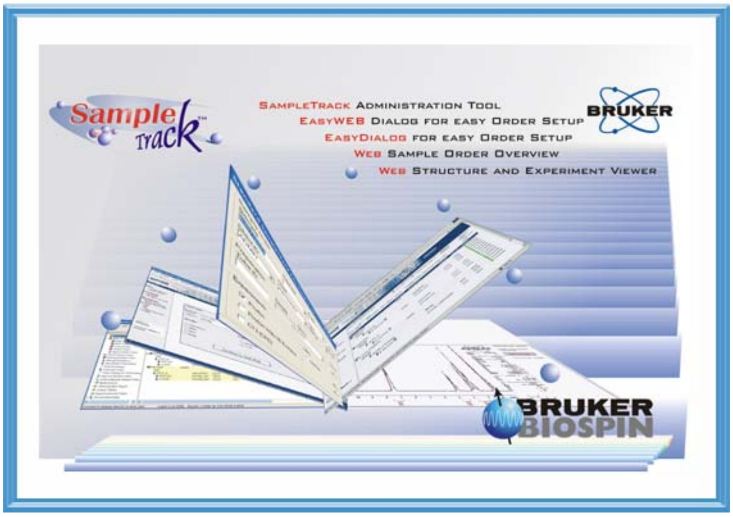
The SampleTrack™ Interfaces 3.3

SampleTrack™ offers a configurable, easy to use interface with all of the features necessary for the administration of day-to-day routine operations in laboratories, such as: sample log-in, bar code printing, report generation, lists of sample submitter's, and lists of sample preparation methods and requested experiments. These features, combined with the underlying database, provide a powerful organizational tool for laboratory managers.

SampleTrack™ is designed to optimize sample tracking, beginning at the submitter's site and continuing through to the final return of results. Information management and hardware control are carried out concurrently as the sample proceeds from the synthesis laboratory through the analytical procedure. Information on the sample is constantly updated and made available to the laboratory personnel as well as to the submitter. Laboratory data is always on-line, active and accessible.

The typical environment of SampleTrack™ is within the NMR laboratory. All work-steps can be processed individually from SampleTrack™ or in conjunction with an external LIMS.

Figure 3.3. The SampleTrack™ Interfaces


SampleTrack
SampleTrack Administration Tool
EasyWEB Dialog for easy Order Setup
EasyDialog for easy Order Setup
Web Sample Order Overview
Web Structure and Experiment Viewer
BRUKER
BRUKER BIOSPIN

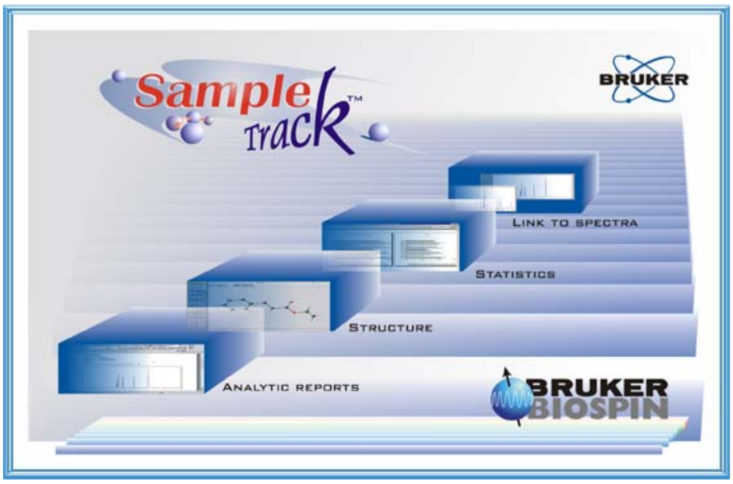
- SampleTrack™ client administration tool ***"SampleTrack™ Environment Setup" on page 85***
- ***"Enter Orders Using the EasyWeb Dialog" on page 76*** for easy order setup in the web
- EasyDialog for easy order setup ***"Introduction to EasyDialog" on page 65***
- ***"WEB Client - Introduction" on page 69***
- ***"Structure and Web Spectra Viewer" on page 72***

SampleTrack™ as Data Reference 3.4

SampleTrack™ consists of a straight forward Client/Server architecture and intuitive user interface within the Microsoft Windows® operating environment. Document usage is easily accomplished through drag & drop selection, and the Client Tool provides easy access to all of your related data (e.g. spectra, structure diagrams, analytical reports etc.)

The SampleTrack™ integrated automation allows you to perform standard and composite experiments without any limitations. And you will have access to your related data even after the archiving process.

Figure 3.4. SampleTrack™ as Data Reference

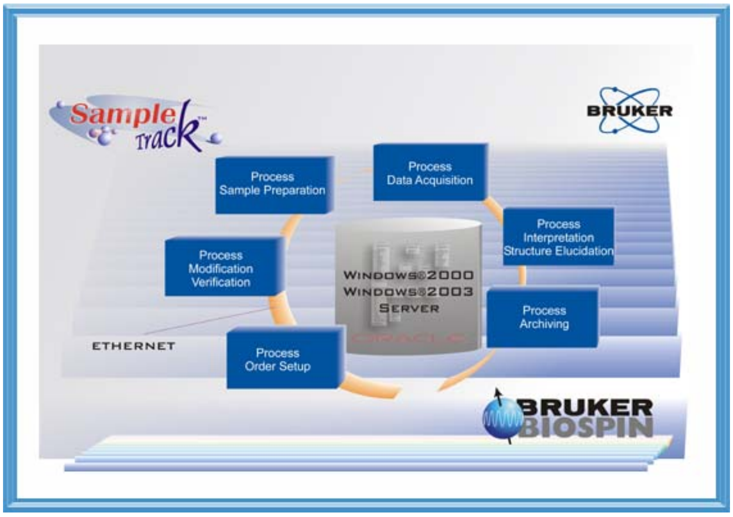


Daily Routine Laboratory Functions *3.5*

In its role as a local management system, SampleTrack™ provides availability for all the daily routine laboratory functions, such as:

- **Order and Report generation**
- **Supervision of the work routine/production**
- **Management of all clients**
- **Preparation methods**
- **The available and permissible experiments**
- **Barcode printing**
- **Order verification**
- **Archiving of all associated data**

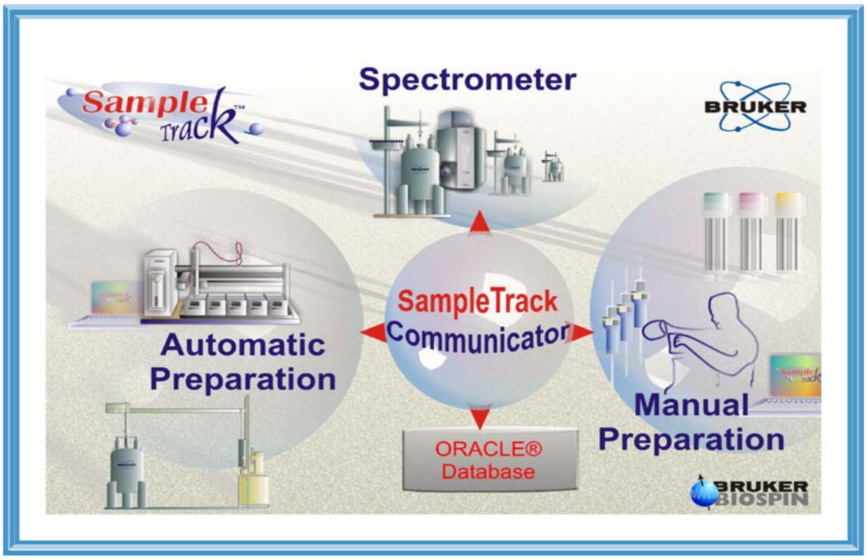
Figure 3.5. Daily Routine Laboratory Functions



Communication Overview 3.6

Orders can be setup with EasyDialog, with the EasyWeb Dialog, within the SampleTrack™ Client, or imported by an external LIMS system. When the status of the manual or automated preparation is set to „finished“, the orders are sent to one of the existing spectrometers, and after measurement, reported back.

Figure 3.6. Communication Overview

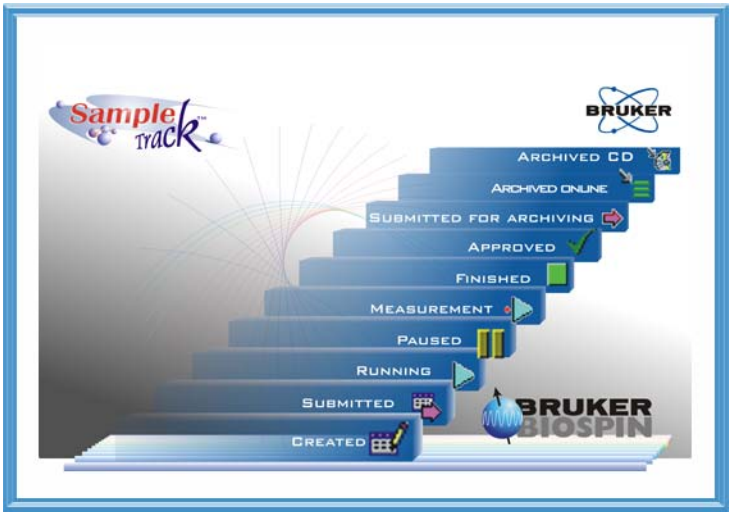


SampleTrack™ Workflow Architecture 3.7

In addition to sample tracking and procedures control, an important feature of SampleTrack™ is the complete recording and documentation of the steps within the procedures. The sample data, path and status, as well as preparation, analysis, spectra transfer and storage are recorded in the local database on the server. This is an essential feature for laboratories operating within GLP regulations.

When no company LIMS is available, laboratory managers can take advantage of the recording and reporting features of SampleTrack™ to document their laboratory studies, in order to utilize them for GLP documentation.

Figure 3.7. SampleTrack™ Workflow Architecture



Integrative Bioinformatics Solution - A Look into the Future 3.8

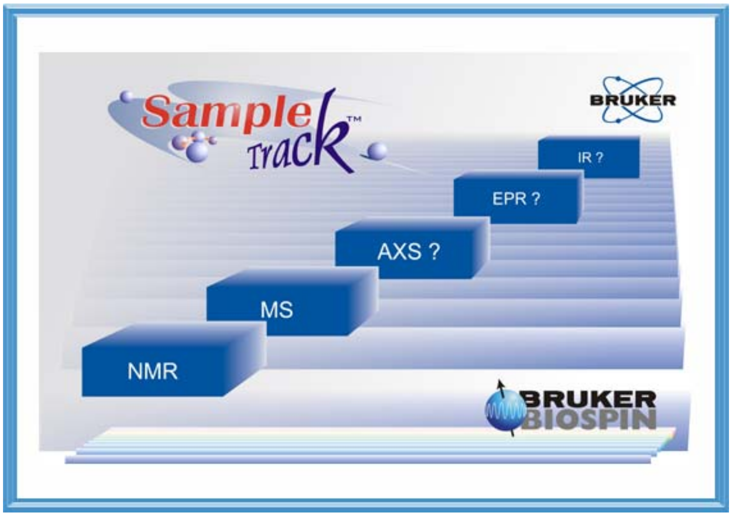
Unique Proteomics RIMS™ integrates multiple information-rich methods (MS/SPR/NMR/XRAY) for increased research productivity in proteomics.

Proteomics RIMS™ combines

- Bruker BioSpin's SampleTrack™ LIMS (Laboratory Information Management System)
- Bruker BioSciences' ProteinScape™ mass spectrometry software
- Bruker AXS X-ray crystallography technologies
- Biacore®'s surface plasmon resonance (SPR) technology for detection and monitoring of biomolecular binding
- Bruker BioSpin's NMR

Dr. Herbert Thiele, Director of Bioinformatics at Bruker Daltonics. "Proteomics RIMS is the logical consequence of Bruker BioSciences and Bruker BioSpin companies providing the entire range of systems solutions for protein MS, x-ray crystallography and NMR. The synergy of their combined and integrated usage is a major step towards increased productivity in drug discovery and target validation."

Figure 3.8. A Look into the Future



Introduction to the SampleTrack™ Client?

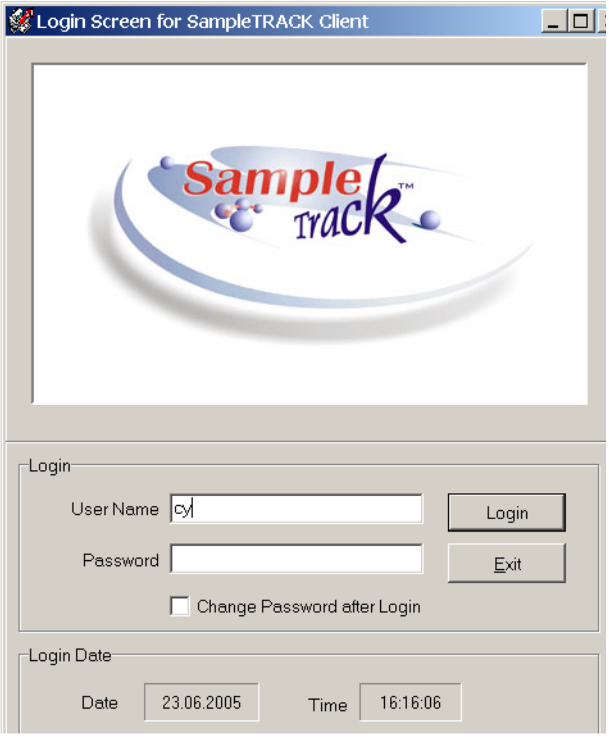
4

SampleTrack™ Login

4.1

When first starting SampleTrack™ Client you will be required to login by entering the appropriate login name and password. The login date and time will be saved at this time.

Figure 4.1. Login Window



Login Screen for SampleTRACK Client

User Name: cy

Password:

☐ Change Password after Login

Login Date

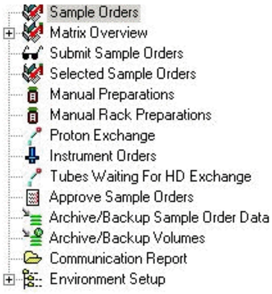
Date: 23.06.2005

Time: 16:16:06

SampleTrack™ Overview *4.2*

On the left side of the main SampleTrack™ Client window is a SampleTrack™ Overview window displayed.

Figure 4.2. Tree Overview



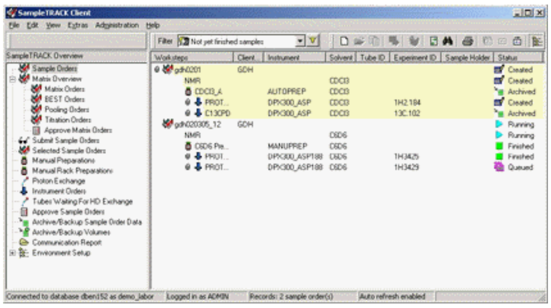
As shown in the figure, this window depicts a tree overview of the various displays that are available. With this overview window, as is customary with most Windows® based applications, the details that are available for each area are displayed when a module is selected. For example, selecting Sample Orders will display all of the current sample overviews that are available.

Sample Orders Module *4.3*

The Sample Orders module provides a good overview of the complete order, without having to change to other parts of the program. All global information, such as Sample ID, Client ID, Instrument, etc., as well as the status of the complete order, are displayed in the Sample Orders heading.

This module also allows you to add, copy and delete sample orders, and to view experiments. You must only click on the corresponding buttons to implement these routines.

Figure 4.3. The Main Window



Worksteps	Client	Instrument	Solvent	Tube ID	Experiment ID	Sample Holder	Status
gdh0201	GDH						Created
NMR			CDCl3				Created
CDCl3_A		AUTOPREP	CDCl3				Archived
PROT...		DPX300_ASP	CDCl3		1H2.184		Created
C13CPD		DPX300_ASP	CDCl3		13C.102		Archived
gdh020305_12	GDH						Running
NMR			C6D6				Running
C6D6 Pre...		MANUPREP	C6D6				Finished
PROT...		DPX300_ASP188	C6D6		1H3425		Finished
PROT...		DPX300_ASP188	C6D6		1H3429		Queued

Connected to database dben152 as demo_labor | Logged in as ADMIN | Records: 2 sample order(s) | Auto refresh enabled

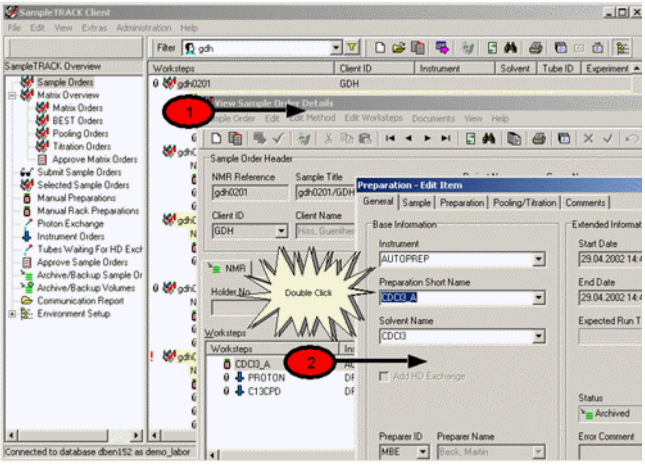
In the NMR method Sample Orders window (shown above), all the worksteps are clearly portrayed within the window. The assignment of individual experiments to the respective preparation steps can be accomplished through inserting appropriate values.

The details of the actual orders are displayed simultaneously in the Sample-Track™ overview window.

Details of a Preparation 4.4

For viewing the details of the individual preparation for a Sample order, double-click on the **Sample ID** line of the menu. This will result in the display of the sample order details window, as shown below.

Figure 4.4. Double Click to See the Sample Order Details

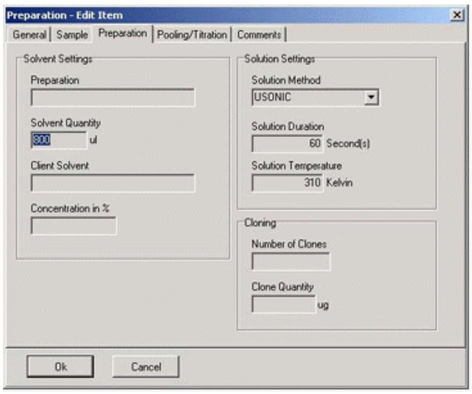


NMR Reference: gdh0201
Sample Title: gdh0201/GDH
Client ID: GDH
Client Name: Hiss, Guenther
Instrument: AUTOPREP
Preparation Short Name: CDCl3_A
Solvent Name: CDCl3
Start Date: 29.04.2002 14:
End Date: 29.04.2002 14:
Expected Run T
Status: Archived
Preparer ID: MBE
Preparer Name: Beck, Martin

Connected to database dben152 as demo_labor

If you wish to view details of an individual experiment, e.g. a preparation, double click on the line of the corresponding preparation workstep. This will display the Preparation Setup window as shown in the figures that follow.

Figure 4.5. Preparation Details

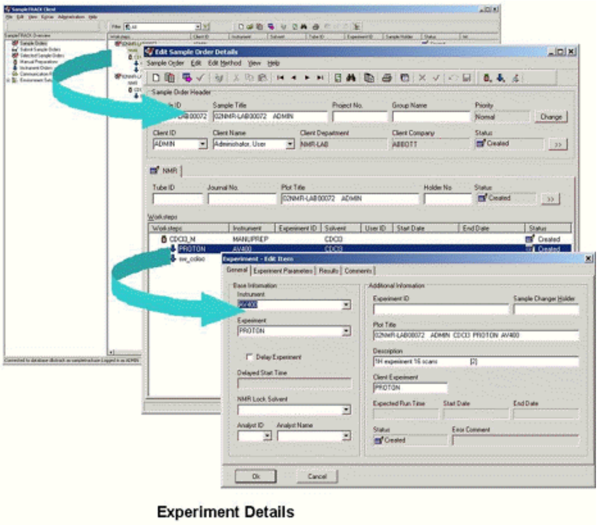


Preparation:
Solvent Quantity: 800 ul
Client Solvent:
Concentration in %:
Solution Method: USONIC
Solution Duration: 60 Second(s)
Solution Temperature: 310 Kelvin
Number of Clones:
Clone Quantity: ug

Sample Order Experiment Details 4.5

You can also view the details of an experiment from the Sample Order Details window by double-clicking on the corresponding workstep.

Figure 4.6. Experiment Details



Sample Order Header

Sample Title: 02NMR-LAB00072 ADMIN
Priority: Normal
Client ID: ADMIN
Client Name: Administrator, User
Client Department: NMR-LAB
Client Company: ABBOTT
Status: Created

NMR

Plot Title: 02NMR-LAB00072 ADMIN
Status: Created

Worksteps

Worksteps	Instrument	Experiment ID	Solvent	User ID	Start Date	End Date	Status
CDCl3_M	MANUPREP		CDCl3				Created
PROTON	AV400		CDCl3				Created

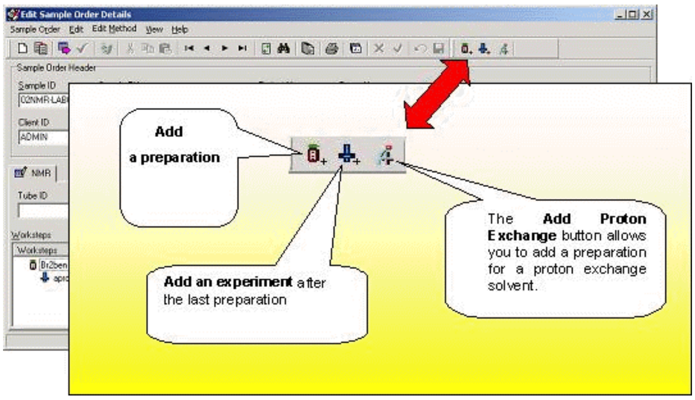
Base Information
Instrument: AV400
Experiment: PROTON
☐ Delay Experiment
Delayed Start Time:
NMR Lock Solvent:
Analyst ID:
Analyst Name:

Additional Information
Experiment ID:
Sample Changer Holder:
Plot Title: 02NMR-LAB00072 ADMIN CDCl3 PROTON AV400
Description: 1H experiment 16 scans [2]
Client Experiment: PROTON
Expected Run Time:
Start Date:
End Date:
Status: Created
Error Comment:

Details Window Buttons *4.6*

On the right edge of the sample order input window you will find **Buttons**, which allow you to quickly add a Preparation, an Experiment or a Proton Exchange.

Figure 4.7. Add Preparation / Experiments / Proton Exchange Buttons



Add
a preparation

Add an experiment after the last preparation

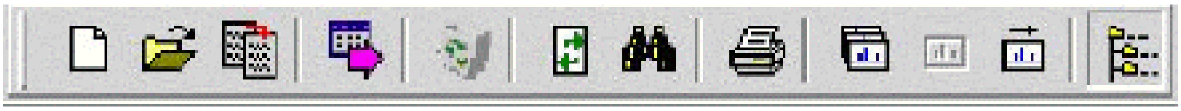
The **Add Proton Exchange** button allows you to add a preparation for a proton exchange solvent.

The **Add Preparation** button allows you to add a new preparation. The **Add Experiment** button allows you to add a new selected experiment The **Add Proton Exchange** button allows you to add a preparation for a proton exchange solvent.

Sample Order Window Buttons 4.7

On top of the Sample Order window you will find **Buttons**, which allow you to quickly select the individual functions for order adjustment and modifications.

Figure 4.8. Sample Order Window Buttons



Create New Sample Order Button

With the Create New Sample Order you can add a complete new order. Pressing this button results in display of a blank Sample Order Details window.

Edit Item Button

The Edit Item button allows you to edit a workstep or the details of an order.

Copy Sample Order Button

With the Copy Sample Order button you may copy an order to form a new one or generate a set of new orders.

Submit Sample Order Button

The Submit Sample Order button is used to begin the measurement, or to restart an experiment with a **Finished** or **Error** status.

Delete Sample Orders Button

With the Delete Sample Orders button you can delete all of the selected sample orders.

Reload or Refresh Button

Reloads the data from the database. This can be automized in the menu Extras.

View all spectra Button

With this button all spectra from one sample order will be displayed.

View Experiment Button

With the View Experiment button you have the possibility of viewing and manipulating the associated spectra of the experiment with an experiment viewer.

View Next Experiment Button

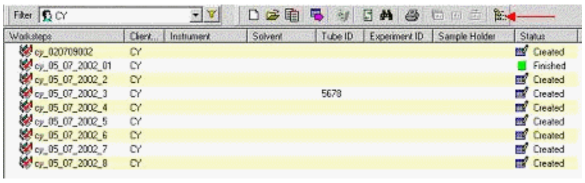
With the View Next Experiment button you can jump to the next existing dataset for viewing or manipulation.

Expand / Contract Button

With the Expand/Contract Button items can be expanded or contracted.

Items expanded

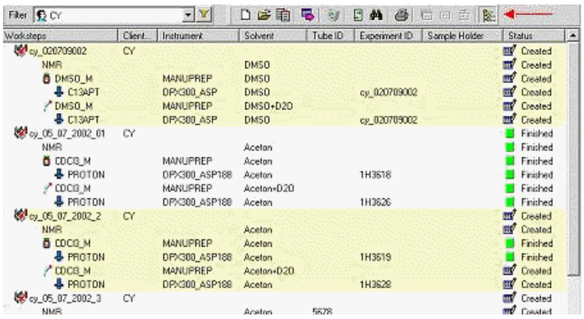
Figure 4.9. Items Contracted



Filter: CY

Worksteps	Client...	Instrument	Solvent	Tube ID	Experiment ID	Sample Holder	Status
cy_020709002	CY						Created
cy_05_07_2002_01	CY						Finished
cy_05_07_2002_2	CY						Created
cy_05_07_2002_3	CY			5678			Created
cy_05_07_2002_4	CY						Created
cy_05_07_2002_5	CY						Created
cy_05_07_2002_6	CY						Created
cy_05_07_2002_7	CY						Created
cy_05_07_2002_8	CY						Created

Figure 4.10. Items Expanded



Filter: CY

Worksteps	Client...	Instrument	Solvent	Tube ID	Experiment ID	Sample Holder	Status
cy_020709002	CY						Created
NMR			DMSO				Created
DMSO_M		MANUPREP	DMSO				Created
C13APT		DPX300_ASP	DMSO		cy_020709002		Created
DMSO_M		MANUPREP	DMSO+D2O				Created
C13APT		DPX300_ASP	DMSO		cy_020709002		Created
cy_05_07_2002_01	CY						Finished
NMR			Aceton				Finished
CDCl3_M		MANUPREP	Aceton				Finished
PROTON		DPX300_ASP188	Aceton		1H3618		Finished
CDCl3_M		MANUPREP	Aceton+D2O				Finished
PROTON		DPX300_ASP188	Aceton		1H3626		Finished
cy_05_07_2002_2	CY						Created
NMR			Aceton				Created
CDCl3_M		MANUPREP	Aceton				Finished
PROTON		DPX300_ASP188	Aceton		1H3619		Finished
CDCl3_M		MANUPREP	Aceton+D2O				Created
PROTON		DPX300_ASP188	Aceton		1H3628		Created
cy_05_07_2002_3	CY						Created
NMR			Aceton	5678			Created

Sample Order Status Information 4.8

In the Sample Orders window it is also possible to receive the complete status information for the selected orders.

Figure 4.11. Status Information

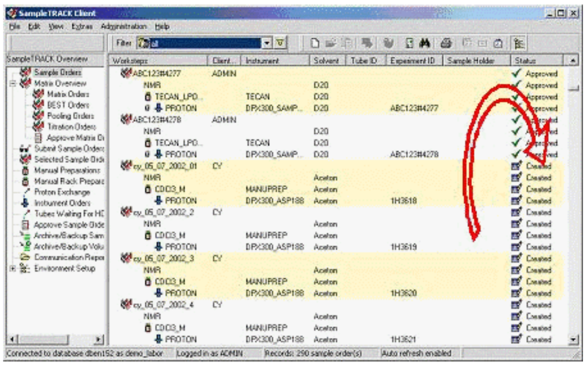
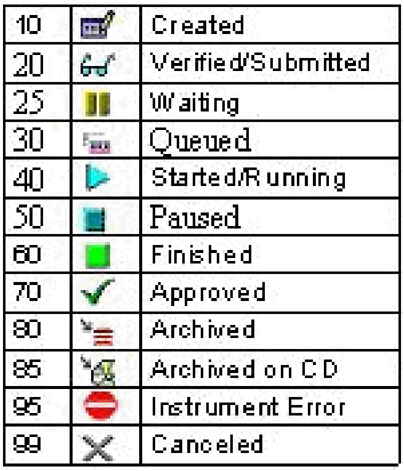


Figure 4.12. List of all Status Symbols



10		Created
20		Verified/Submitted
25	⏸	Waiting
30		Queued
40	▶	Started/Running
50	■	Paused
60	🟩	Finished
70	✓	Approved
80		Archived
85		Archived on CD
95	⛔	Instrument Error
99	✗	Canceled

Filters & Views 4.9

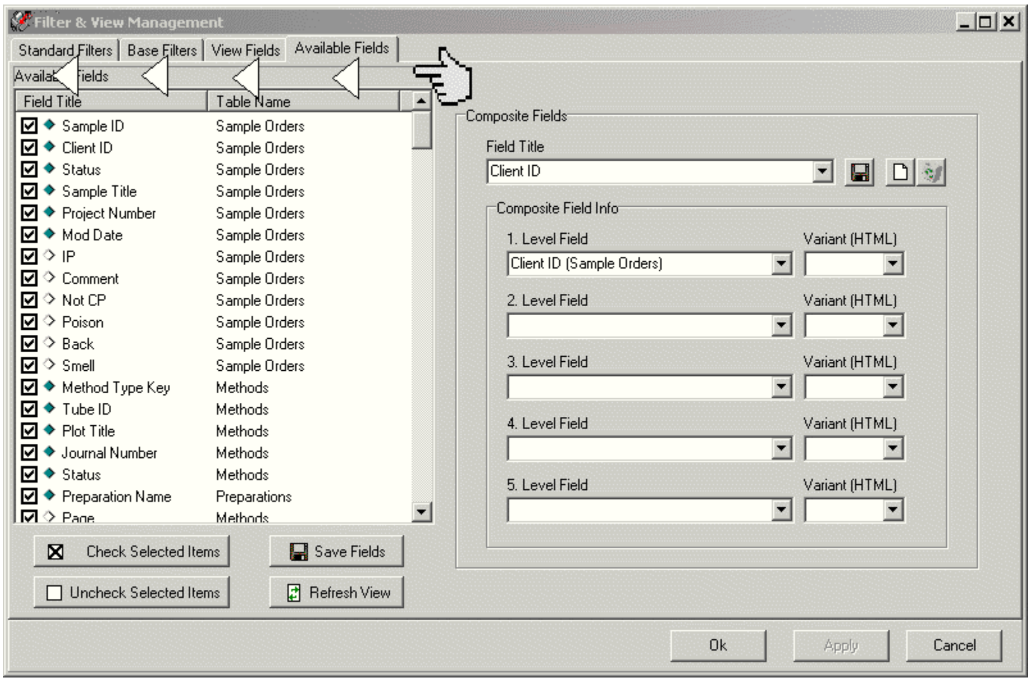
Specific client or department fields and their views are managed by the filter & view assistant.

Figure 4.13. Filter & View Assistant Button

Basic filters select only those orders which the user or their department are principally allowed to see.

Within this personal data pool **user specific filters** can be set.

Figure 4.14. Filter and view management



	Field Title	Table Name
☑	◆ Sample ID	Sample Orders
☑	◆ Client ID	Sample Orders
☑	◆ Status	Sample Orders
☑	◆ Sample Title	Sample Orders
☑	◆ Project Number	Sample Orders
☑	◆ Mod Date	Sample Orders
☑	◇ IP	Sample Orders
☑	◇ Comment	Sample Orders
☑	◇ Not CP	Sample Orders
☑	◇ Poison	Sample Orders
☑	◇ Back	Sample Orders
☑	◇ Smell	Sample Orders
☑	◆ Method Type Key	Methods
☑	◆ Tube ID	Methods
☑	◆ Plot Title	Methods
☑	◆ Journal Number	Methods
☑	◆ Status	Methods
☑	◆ Preparation Name	Preparations
☑	◇ Page	Methods

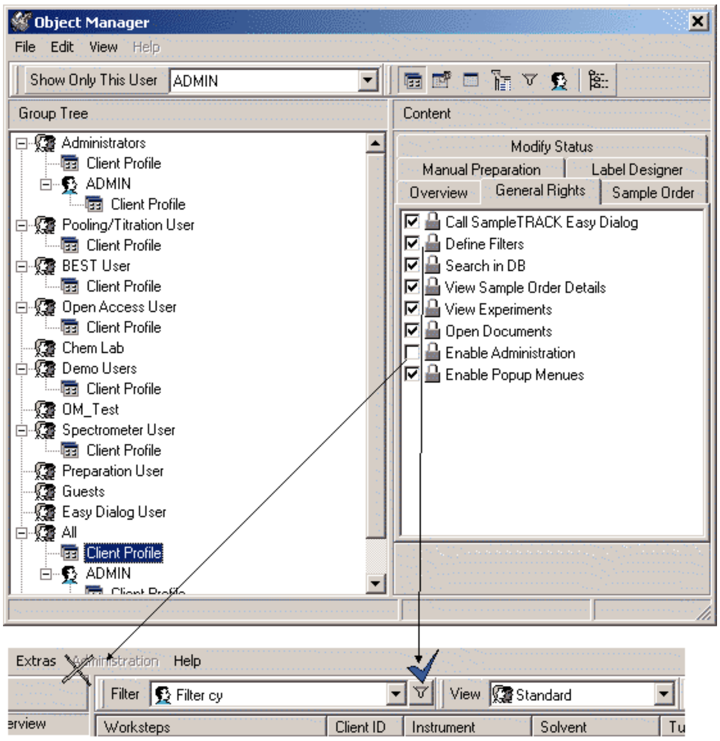
Field Title: Client ID

1. Level Field: Client ID (Sample Orders) Variant (HTML):
2. Level Field: Variant (HTML):
3. Level Field: Variant (HTML):
4. Level Field: Variant (HTML):
5. Level Field: Variant (HTML):

The Right to Define Filters *4.9.1*

The users might be allowed to define their standard filters but are not allowed to define basic filters and available fields. In order to use this option, the necessary user privileges must first be assigned by the Administrator in the Object Manager as shown below.

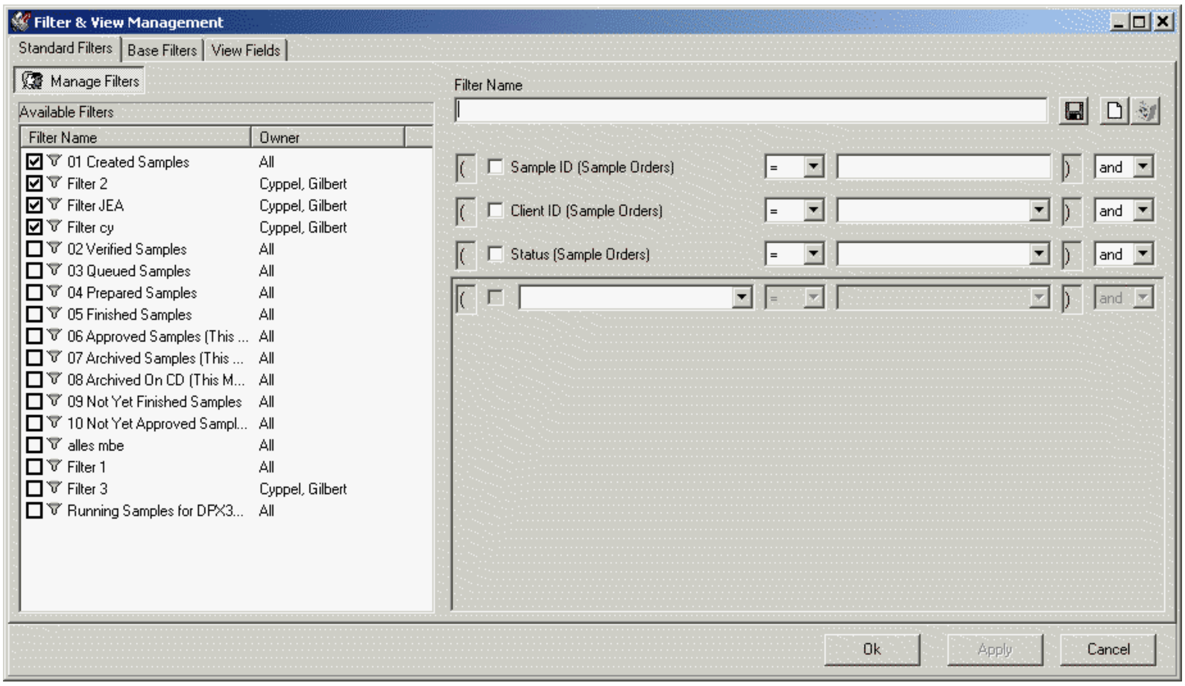
Figure 4.15. The Object Manager



☑ Call SampleTRACK Easy Dialog
☑ Define Filters
☑ Search in DB
☑ View Sample Order Details
☑ View Experiments
☑ Open Documents
☐ Enable Administration
☑ Enable Popup Menues

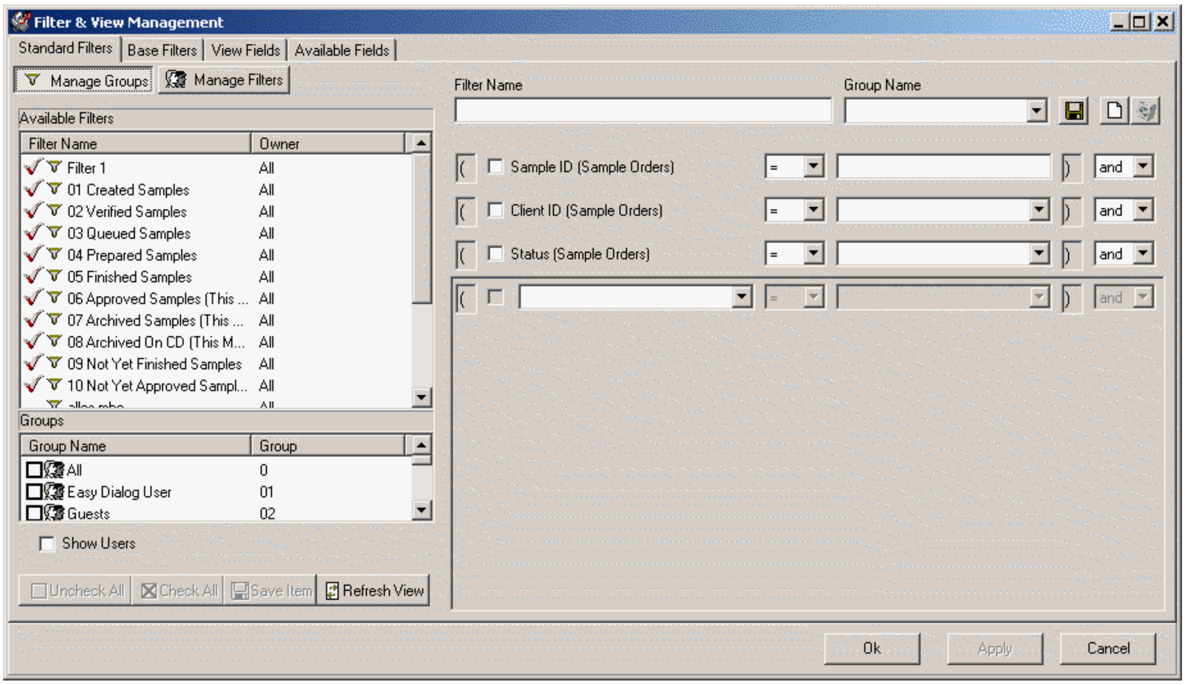
When the **Define Filter** box is checked and the **Enable Administration** box unchecked as in the example above, the user only has minimal rights to define their personal views and filters.

Figure 4.16. Filter Management


Filter & View Management
Standard Filters
Base Filters
View Fields
Manage Filters
Available Filters
Filter Name
Owner
☑ 01 Created Samples All
☑ Filter 2 Cyppel, Gilbert
☑ Filter JEA Cyppel, Gilbert
☑ Filter cy Cyppel, Gilbert
☐ 02 Verified Samples All
☐ 03 Queued Samples All
☐ 04 Prepared Samples All
☐ 05 Finished Samples All
☐ 06 Approved Samples (This ... All
☐ 07 Archived Samples (This ... All
☐ 08 Archived On CD (This M... All
☐ 09 Not Yet Finished Samples All
☐ 10 Not Yet Approved Sampl... All
☐ alles mbe All
☐ Filter 1 All
☐ Filter 3 Cyppel, Gilbert
☐ Running Samples for DPX3... All
Filter Name
(☐ Sample ID (Sample Orders) =) and
(☐ Client ID (Sample Orders) =) and
(☐ Status (Sample Orders) =) and
(☐ =) and
Ok
Apply
Cancel

When the **Define Filter** box and the **Enable Administration** box are checked, which is usually a privilege for the administrator, the entire functionality is available:

Figure 4.17. Filter Management



For further information see ***"Filter and Search Tools" on page 54*** and ***"Inserting a New Filter Method" on page 109***

Functions of the SampleTrack™ Client Module

5

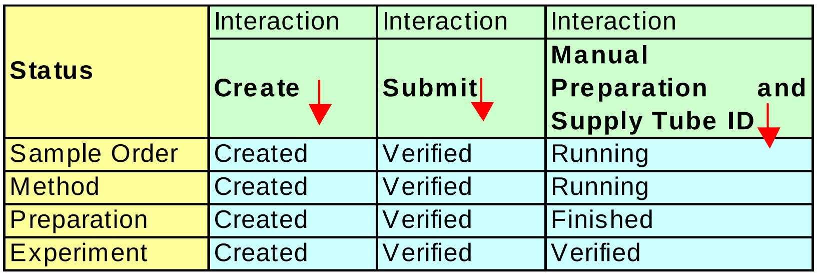
Submit Sample Orders

5.1

Depending on the workflow in the laboratory, the order must be handled by the official person or set automatically by the SampleTrack™ system.

In the following scenario the order is verified manually. After creating an order using EasyDialog or within the client the status of the order remains **Created**.

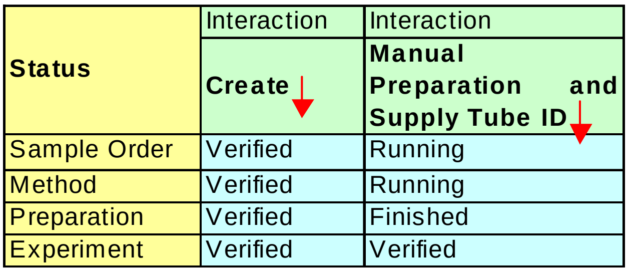
Figure 5.1. Scenario 1



Status	Interaction	Interaction	Interaction
	Create ↓	**Submit** ↓	**Manual Preparation and Supply Tube ID** ↓
Sample Order	Created	Verified	Running
Method	Created	Verified	Running
Preparation	Created	Verified	Finished
Experiment	Created	Verified	Verified

In the next scenario the step **Submit Order** is skipped, whereas the next step is the **Manual Preparation**:

Figure 5.2. Scenario 2



Status	Interaction	Interaction
	Create ↓	**Manual Preparation and Supply Tube ID** ↓
Sample Order	Verified	Running
Method	Verified	Running
Preparation	Verified	Finished
Experiment	Verified	Verified

Another scenario could be a LIMS Import by an external LIMS workaround with prepared NMR samples:

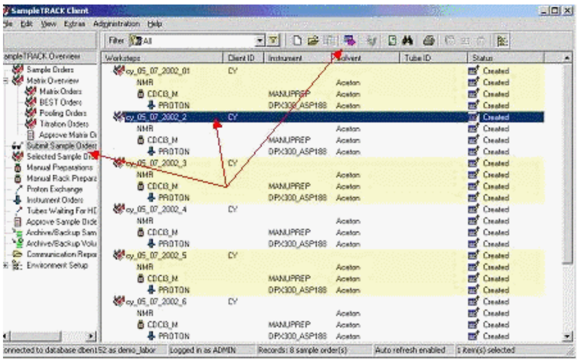
Figure 5.3. Scenario 3

Status	Interaction	Interaction
	Sample Orders ↓ by LIMS	**Submit** ↓
Sample Order	Created	Running
Method	Created	Running
Preparation	Finished	Finished
Experiment	Created	Verified

A completely automized workaround, without interaction, is possible when the orders are imported and immediately submitted by the system.

The area Submit Sample Orders on the left side provides a method of displaying an overview of the manually created and/or imported orders, and sample orders with an **Error** status.

Figure 5.4. Status Overview

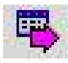


Worksteps	Client ID	Instrument	Solvent	Tube ID	Status
cy_05_07_2002_01	CY				Created
NMR			Aceton		Created
CDCl3_M		MANUPREP	Aceton		Created
PROTON		DPX300_ASP188	Aceton		Created
cy_05_07_2002_2	CY				Created
NMR			Aceton		Created
CDCl3_M		MANUPREP	Aceton		Created
PROTON		DPX300_ASP188	Aceton		Created
cy_05_07_2002_3	CY				Created
NMR			Aceton		Created
CDCl3_M		MANUPREP	Aceton		Created
PROTON		DPX300_ASP188	Aceton		Created
cy_05_07_2002_4	CY				Created
NMR			Aceton		Created
CDCl3_M		MANUPREP	Aceton		Created
PROTON		DPX300_ASP188	Aceton		Created
cy_05_07_2002_5	CY				Created
NMR			Aceton		Created
CDCl3_M		MANUPREP	Aceton		Created
PROTON		DPX300_ASP188	Aceton		Created
cy_05_07_2002_6	CY				Created
NMR			Aceton		Created
CDCl3_M		MANUPREP	Aceton		Created
PROTON		DPX300_ASP188	Aceton		Created

onnected to database dben152 as demo_labor | Logged in as ADMIN | Records: 8 sample order(s) | Auto refresh enabled | 1 item(s) selected

The orders can be verified from here using the **Submit** button.

Figure 5.5. The Submit Button



Select All - use the right mouse click to mark all of the orders as **Submitted**

Figure 5.6. Select All

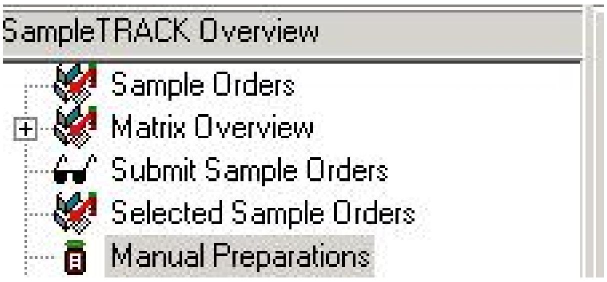
Select All Strg+A

When a modification of an order is necessary, you can automatically move to the Sample Order Details window by double-clicking on the order.

Manual Preparation *5.2*

This module is used by the preparation work area. Orders must have a submitted/ verified status in order for the Sample ID to be reported here.

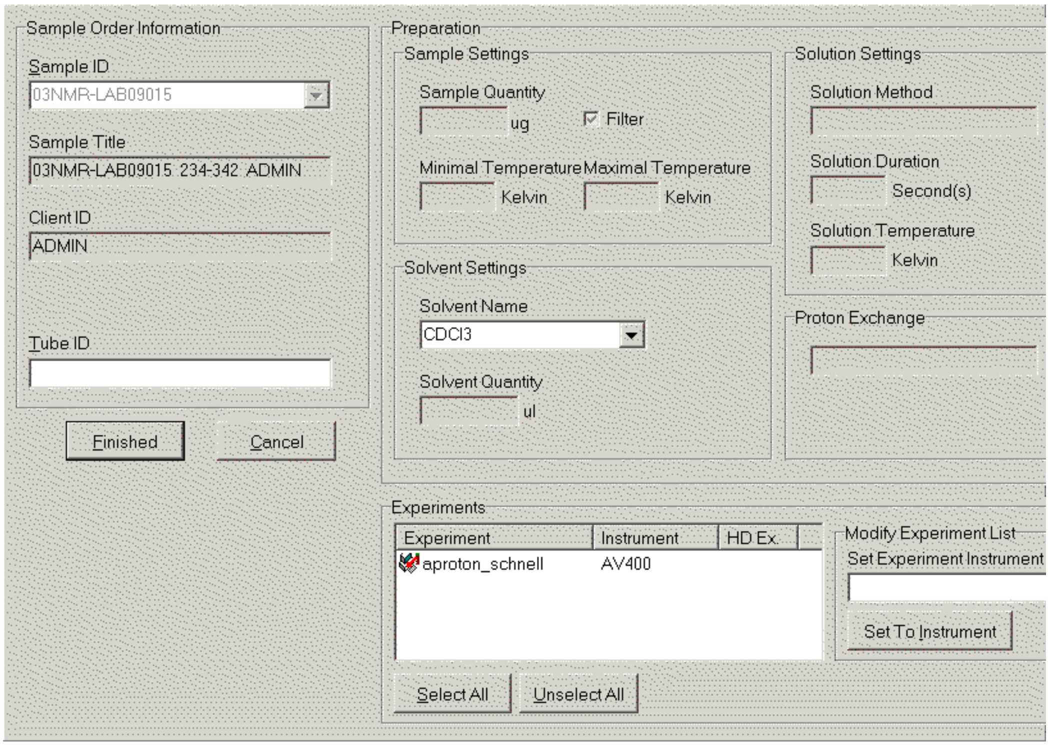
Figure 5.7. Tree - Manual Preparation Area



The goal of this module is that the preparer needs only to provide the minimum information necessary to confirm the implemented preparation and with it the generation of the necessary instrument order.

To display the respective preparation data of an order in the Manual Preparation window, the Sample ID should first be selected by using a barcode reader, by entering the ID number manually, or by selecting the ID number from a pull-down menu.

Figure 5.8. The Manual Preparation Window



Sample ID: 03NMR-LAB09015

Sample Title: 03NMR-LAB09015 234-342 ADMIN

Client ID: ADMIN

☑ Filter

Solvent Name: CDCl3

Experiment	Instrument	HD Ex.
aproton_schnell	AV400	

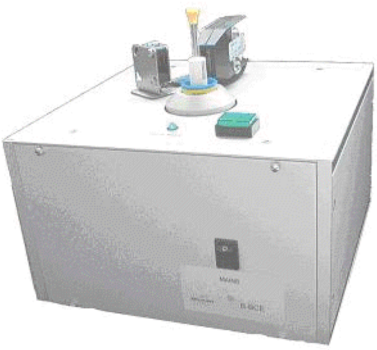
If the solvent that has been selected is not applicable, a different solvent can be selected from this dialog window.

The instrument that is used for the experiment can also be selected or changed in this window.

Once the preparation has been performed and the barcode collar placed on the tube, the Tube ID from this collar must be entered in the Tube ID block in the Manual Preparation window.

After assigning a Tube ID, the order is **submitted** by pressing the **Finished** button.

Figure 5.9. B-BCE for Easy Tube ID Barcode Reading



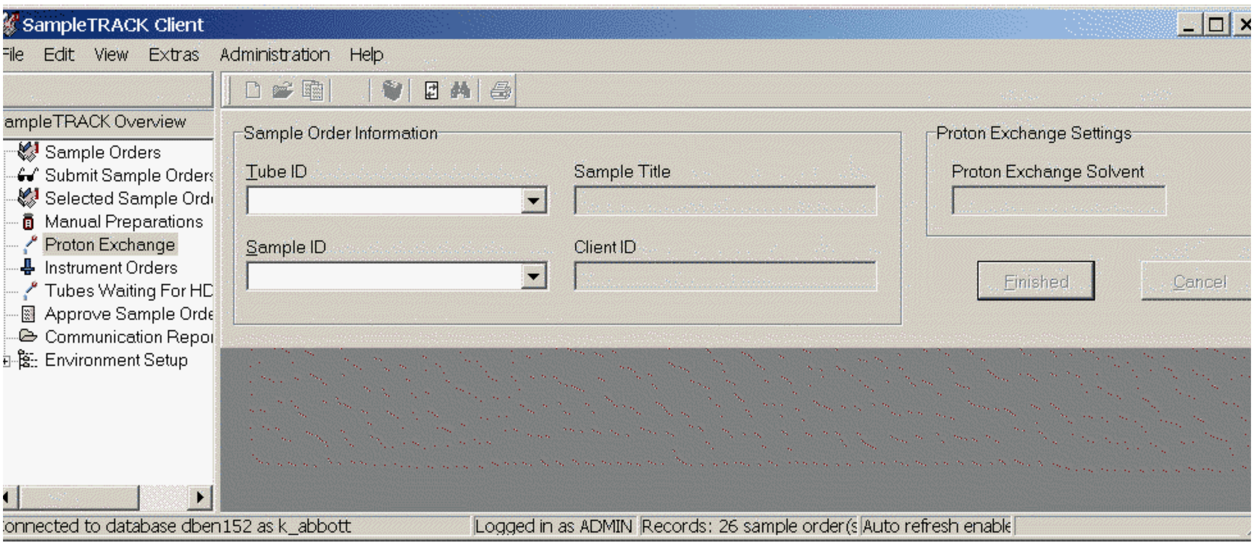
An instrument often used for this purpose, the B-BCE, is connected with the computer and can automatically fulfill this procedure.

Proton Exchange 5.3

This module has been created to give the preparer the possibility of searching for an order associated with a sample tube ID.

After the preparer adds the proton exchange solvent to the sample in the lab, the new order for the spectrometer is automatically generated by pressing the Finished button.

Figure 5.10. The Proton Exchange Window



onnected to database dben152 as k_abbott | Logged in as ADMIN | Records: 26 sample order(s | Auto refresh enable

Finish Manual Experiments 5.4

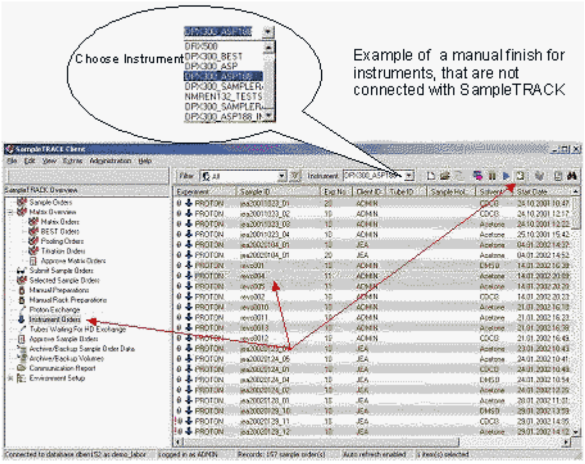
When experiments from a sample order have been measured on an instrument which is **not connected** to the SampleTrack™ system it is necessary to manually set the status of the experiment to **Finished.** This is necessary to be able to use the Order Approval window to approve the orders and release the Tube ID for re-use.

Figure 5.11. The Finished Button

When you press the Finished button, all selected experiments are set to the **Finished** status. If all experiments in an order have been completed, the complete sample order is also set to **Finished**.

You are then able to use the **Order Approval** window to approve the orders and release the Tube ID.

Figure 5.12. Example of a Manual Implemented Finish



Example of a manual finish for instruments, that are not connected with SampleTRACK

Delay Experiments 5.5

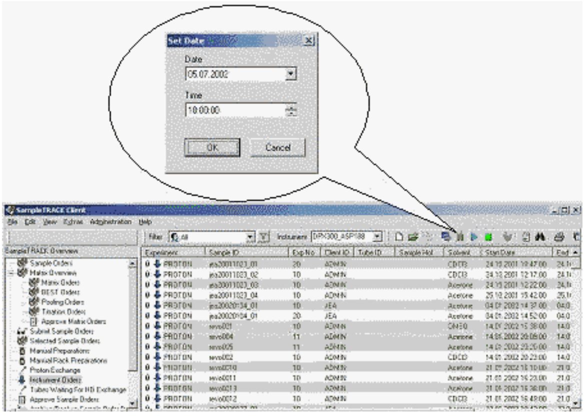
In some cases it is desirable to delay the measurement from a specific experiment or experiment set. For example, to allow all C13 experiments to be run over the night or weekend in order to save the spectrometer time for proton experiments during the day.

Figure 5.13. Status Icon of Waiting / Delayed Experiments t

⏸

The Delay Experiments window and its button allows you to set these experiments to the **Delayed** status for processing at a later time. The pull-down menu **Experiment Type** allows you to select various experiment types (nucleus). Experiments that have been delayed have a **Waiting** status.

Figure 5.14. Delay Experiments



Date: 05.07.2002

Time: 10:00:00

Experiments Waiting (Delayed) 5.6

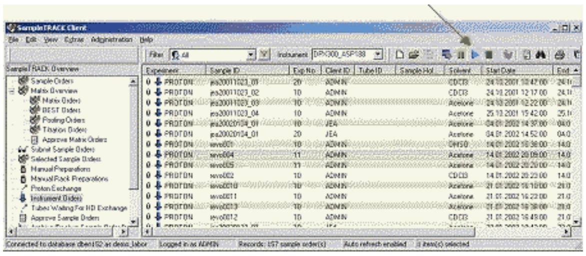
The **Start** the button within the Instrument Orders Window used to start the measurement of **Waiting (delayed)** status experiments.

Figure 5.15. The Start Delayed Experiments Button

To start the experiment you must only highlight an experiment and press the **Start Experiment** button. If you have multiple experiments you can check the **Start Box** to the right of the desired experiments (or use **Select All** to select all of the experiments) and then press the **Start Experiment** button to begin the experiments.

You can also edit a selected sample order from this window, before starting the experiment, by pressing the **Edit Sample Order** button.

Figure 5.16. Highlight and Start Delayed Experiments

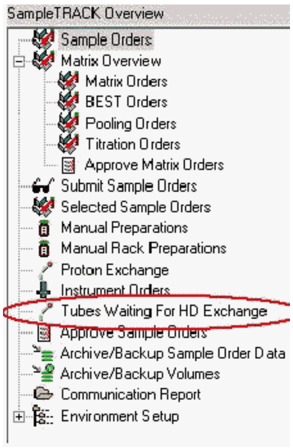


Connected to database dben152 as demo_labor | Logged in as ADMIN | Records: 157 sample order(s) | Auto refresh enabled | 0 item(s) selected

Experiments Waiting for HD Exchange 5.7

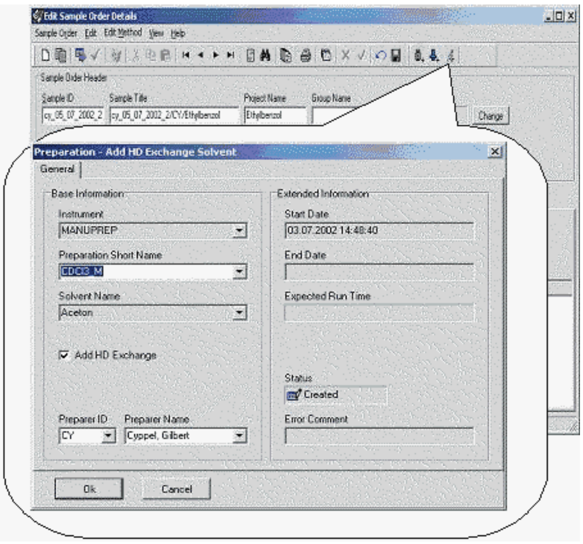
This module is NMR specific. In this window all of the orders that are waiting for the addition of the solvent for the proton hydrogen/deuterium exchange can be viewed or printed out in report form. As with the Experiments Waiting (Delayed) you can also edit a sample order from this window.

Figure 5.17. Tubes Waiting for HD Exchange



The HD Exchange Solvent window is opened in the detail window using the folowing button

Figure 5.18. The HD Exchange Window



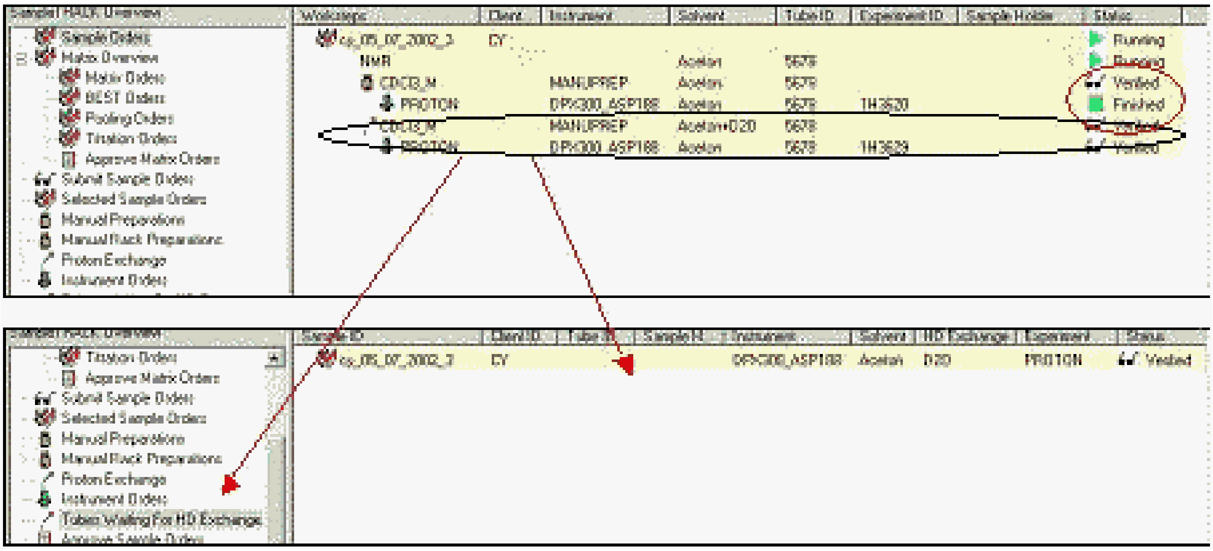
Sample ID: cy_05_07_2002_2
Sample Title: cy_05_07_2002_2/CY/Ethylbenzol
Project Name: Ethylbenzol

Instrument: MANUPREP
Preparation Short Name: CDCl3_M
Solvent Name: Aceton
☑ Add HD Exchange
Preparer ID: CY
Preparer Name: Cyppel, Gilbert

Start Date: 03.07.2002 14:48:40
End Date:
Expected Run Time:
Status: Created
Error Comment:

When the previous experiment within the order is finished, the exchange experiment can be found and handled in the **Tubes Waiting for Exchange** window.

Figure 5.19. The Tubes Waiting for Exchange Window



Worksteps	Client	Instrument	Solvent	Tube ID	Experiment ID	Sample Holder	Status
cq_05_07_2002_3	CY						Running
NMR			Aceton	5678			Running
CDCl3_M		MANUPREP	Aceton	5678			Verified
PROTON		DPX300_ASP188	Aceton	5678	1H3620		Finished
CDCl3_M		MANUPREP	Aceton+D20	5678			Verified
PROTON		DPX300_ASP188	Aceton	5678	1H3629		Verified

Sample ID	Client ID	Tube #	Sample H	Instrument	Solvent	HD Exchange	Experiment	Status
cq_05_07_2002_3	CY			DPX300_ASP188	Aceton	D2O	PROTON	Verified

Order Approval 5.8

The Order Approval module allows you to approve finished orders so that you can **reuse Tube ID barcode collars**. Individual reports can also be generated for viewing or printing by using corresponding filters.

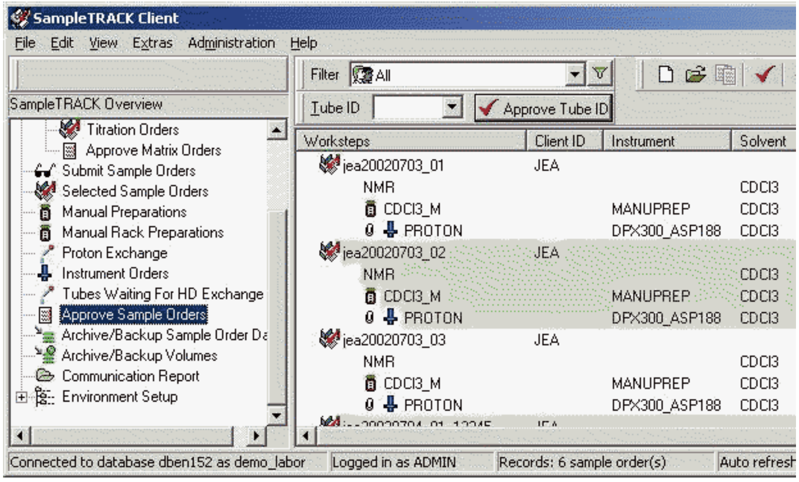
With this module you may approve all finished orders at once (Select All / CTRL A) or you may select orders individually by clicking on the **Approved** box with your mouse.

To reverse the **Select All** process, press Refresh, which will remove the check-marks.

Through this process the header status is set to approved and the Tube ID is removed from the valid data field releasing it for reuse.

Once the order has the **Approved** status, no other changes are possible, unless the order is not reset.

Figure 5.20. The Approve Window



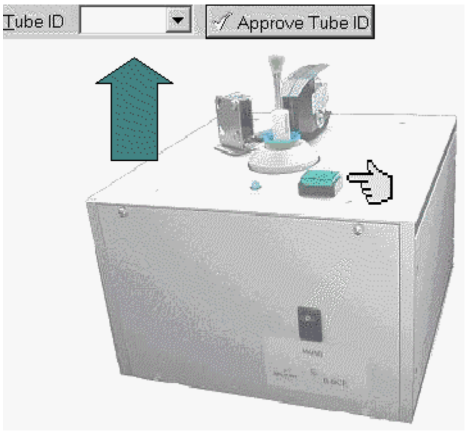
Filter: All

Worksteps	Client ID	Instrument	Solvent
jea20020703_01	JEA		
NMR			CDCl3
CDCl3_M		MANUPREP	CDCl3
PROTON		DPX300_ASP188	CDCl3
jea20020703_02	JEA		
NMR			CDCl3
CDCl3_M		MANUPREP	CDCl3
PROTON		DPX300_ASP188	CDCl3
jea20020703_03	JEA		
NMR			CDCl3
CDCl3_M		MANUPREP	CDCl3
PROTON		DPX300_ASP188	CDCl3

Connected to database dben152 as demo_labor | Logged in as ADMIN | Records: 6 sample order(s) | Auto refresh

The B-BCE can be used to easily approve an order and release the Tube ID.

Figure 5.21. B-BCE



E-mail Notification *5.9*

It is also possible to provide automatic customer notification via E-mail , when the order is complete.

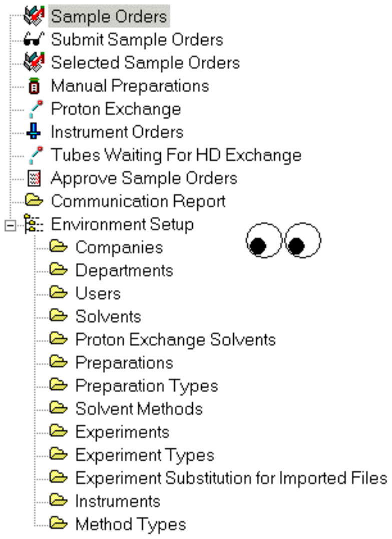
With this E-mail it is possible to send the spectra data as an attachment.

See also: ***"E-Mail Support" on page 137***

Environment Setup *5.10*

The Environment Setup depicts the area, where all of the adjustments and definitions for the complete system environment are implemented. Refer to the Sample-Track Environment for further information ***"SampleTrack™ Environment Setup" on page 85***.

Figure 5.22. The Environment Setup Area



- Sample Orders
- Submit Sample Orders
- Selected Sample Orders
- Manual Preparations
- Proton Exchange
- Instrument Orders
- Tubes Waiting For HD Exchange
- Approve Sample Orders
- Communication Report
- Environment Setup
  - Companies
  - Departments
  - Users
  - Solvents
  - Proton Exchange Solvents
  - Preparations
  - Preparation Types
  - Solvent Methods
  - Experiments
  - Experiment Types
  - Experiment Substitution for Imported Files
  - Instruments
  - Method Types

Working with the SampleTrack™ Client

6

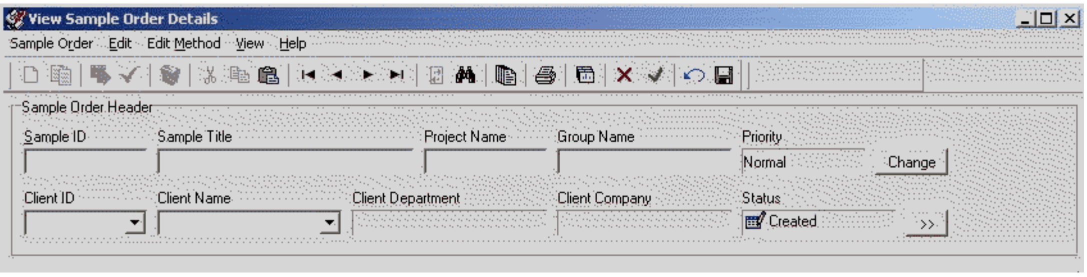
Sample Order Details Window 6.1

To set up a sample order move to the Sample Order window and press the Add Sample Order button.

🗋

This will open a new, empty Sample Order Details window.

Figure 6.1. SampleTrack Order



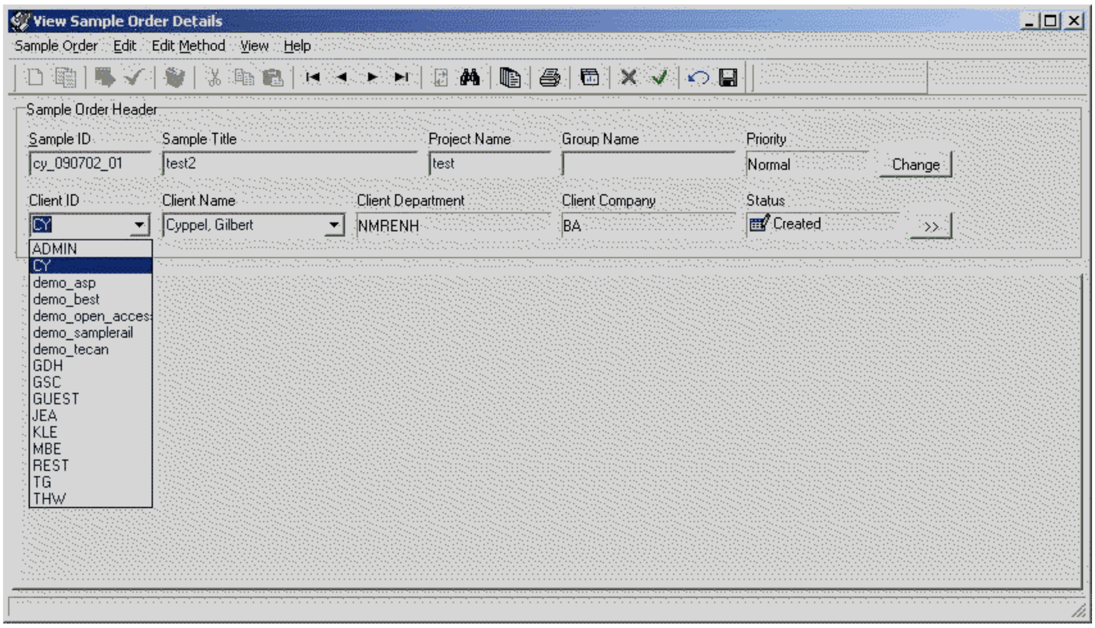
Priority: Normal

Status: Created

Entering the Sample and Client ID 6.2

Enter your Sample ID and optionally a Project No. and Group ID. Using the TAB key or mouse move to the client ID field and enter the Client ID, or select it from the list of values from the pull-down menu.

Figure 6.2. Entering the Client ID

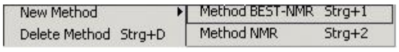


Sample ID: cy_090702_01
Sample Title: test2
Project Name: test
Group Name:
Priority: Normal
Client ID: CY
Client Name: Cyppel, Gilbert
Client Department: NMRENH
Client Company: BA
Status: Created

Define a Method and Enter the Journal Number 6.3

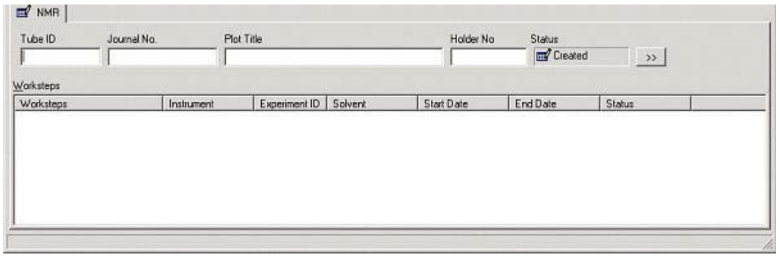
To define a method like NMR, BEST, … click the right mouse button:

Figure 6.3. Defining a New Method Using Right Mouse Button



or press Ctrl 1, Ctrl 2, …

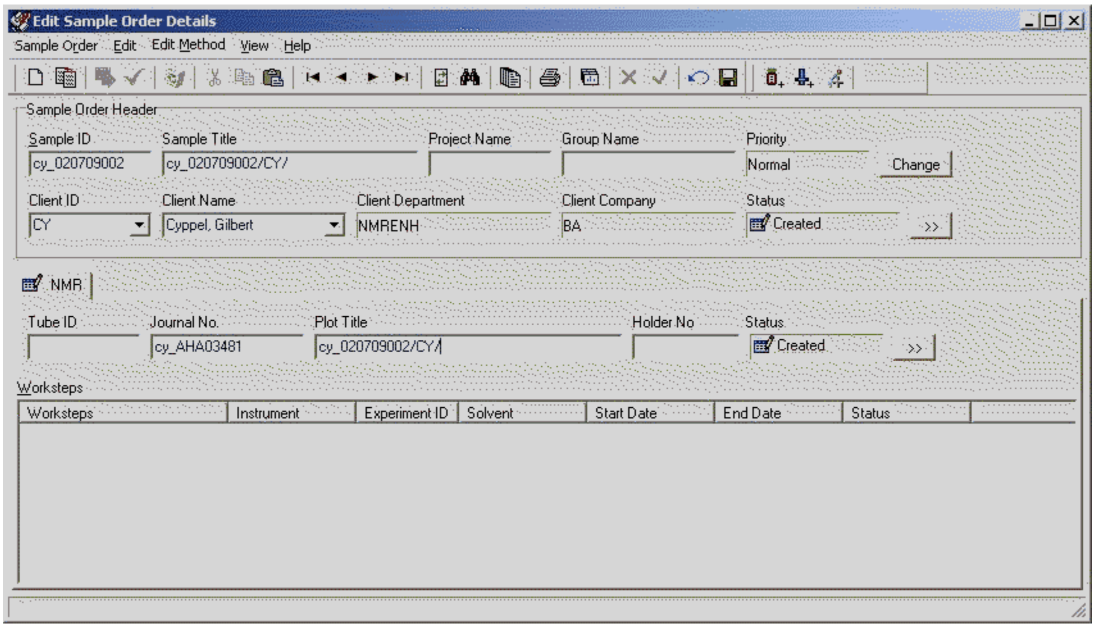
Figure 6.4. Entering the Journal Number



Optionally enter your journal number in the Journal No. block. As you move to this block the header of the order is automatically stored in the database.

When you save the order the **Edit Sample Order Details** window will appear.

Figure 6.5. The Edit Sample Order Details Window



Sample ID: cy_020709002
Sample Title: cy_020709002/CY/
Project Name:
Group Name:
Priority: Normal
Client ID: CY
Client Name: Cyppel, Gilbert
Client Department: NMRENH
Client Company: BA
Status: Created

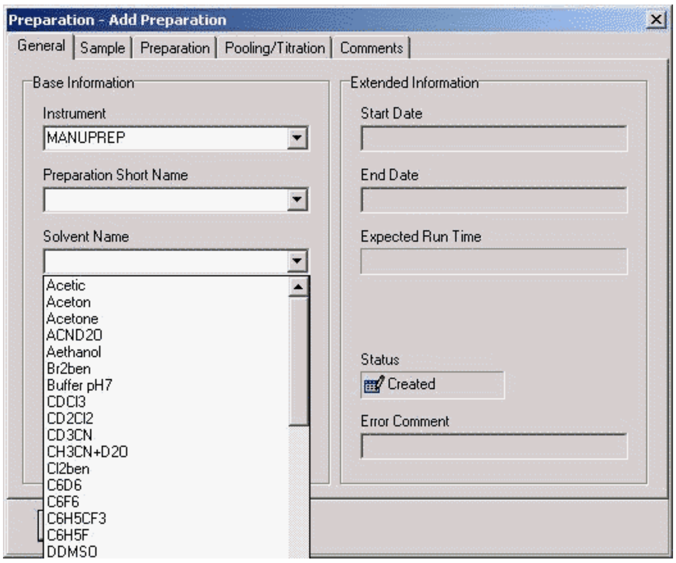
Tube ID:
Journal No.: cy_AHA03481
Plot Title: cy_020709002/CY/
Holder No:
Status: Created

Worksteps	Instrument	Experiment ID	Solvent	Start Date	End Date	Status

Select the Preparation Workstep 6.4

Move to the Worksteps block and press the Add Preparation button to enter the necessary preparation. A Preparation Setup window will be opened, whereby you can select the desired preparation from the pull-down list of available preparations located under the Preparation block.

Figure 6.6. Select a Preparation



Instrument: MANUPREP
Preparation Short Name:
Solvent Name:

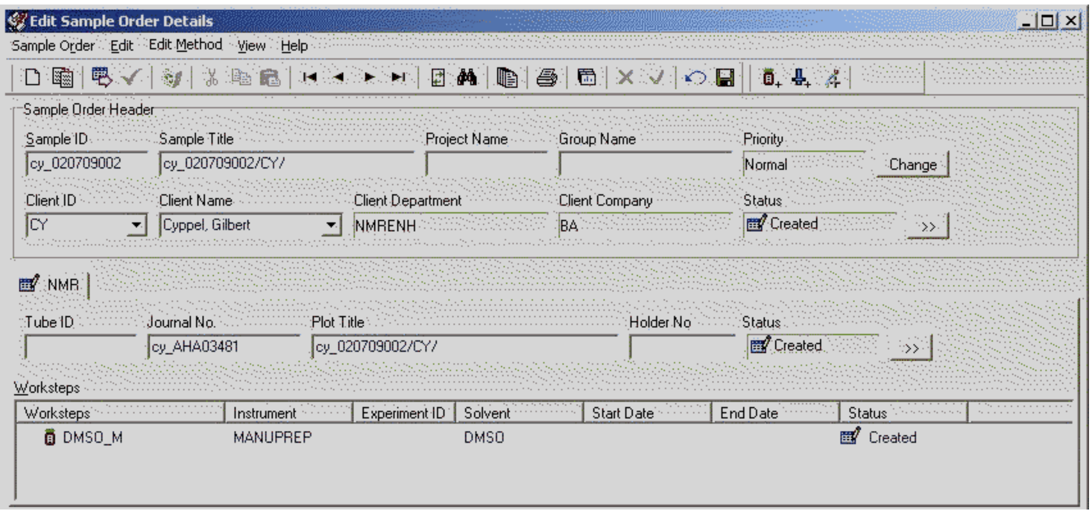
Acetic
Aceton
Acetone
ACND2O
Aethanol
Br2ben
Buffer pH7
CDCl3
CD2Cl2
CD3CN
CH3CN+D2O
Cl2ben
C6D6
C6F6
C6H5CF3
C6H5F
DDMSO

Start Date:
End Date:
Expected Run Time:
Status: Created
Error Comment:

Upon selection of a preparation, all predefined values will be displayed. You may modify them as needed, or accept the values by pressing the OK button.

The preparation entry is now complete and will be displayed as a workstep in your order. The Sample Title and Plot Title is automatically created, using your pre-defined function, and entered in the database.

Figure 6.7. Order Details



Sample ID: cy_020709002
Sample Title: cy_020709002/CY/
Project Name:
Group Name:
Priority: Normal
Client ID: CY
Client Name: Cyppel, Gilbert
Client Department: NMRENH
Client Company: BA
Status: Created

NMR
Tube ID:
Journal No.: cy_AHA03481
Plot Title: cy_020709002/CY/
Holder No:
Status: Created

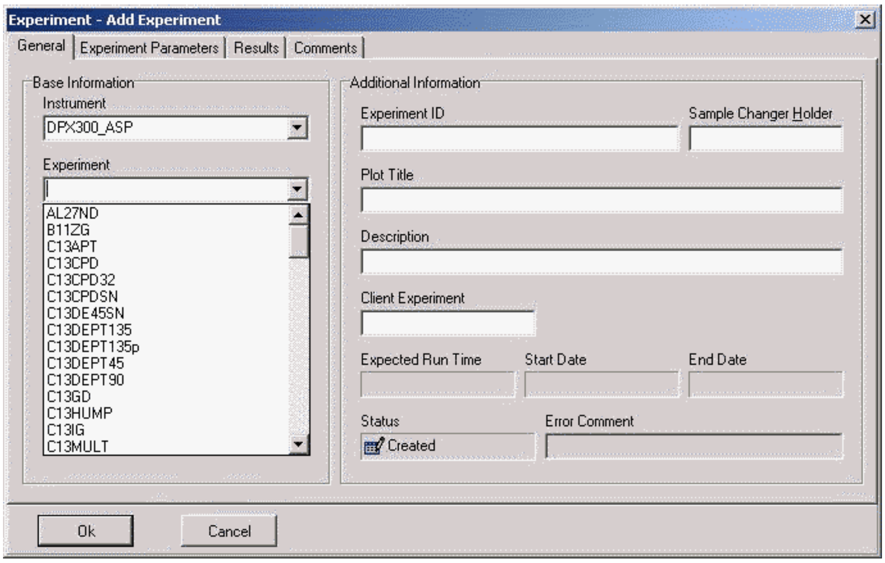
Worksteps	Instrument	Experiment ID	Solvent	Start Date	End Date	Status
DMSO_M	MANUPREP		DMSO			Created

Adding Experiments 6.5

Your order is now ready for you to define the experiments that are planned. Press the button Add Experiment.

A window for inserting new experiments will be opened.

Figure 6.8. Add Experiment



Instrument: DPX300_ASP
Experiment:
AL27ND
B11ZG
C13APT
C13CPD
C13CPD32
C13CPDSN
C13DE45SN
C13DEPT135
C13DEPT135p
C13DEPT45
C13DEPT90
C13GD
C13HUMP
C13IG
C13MULT

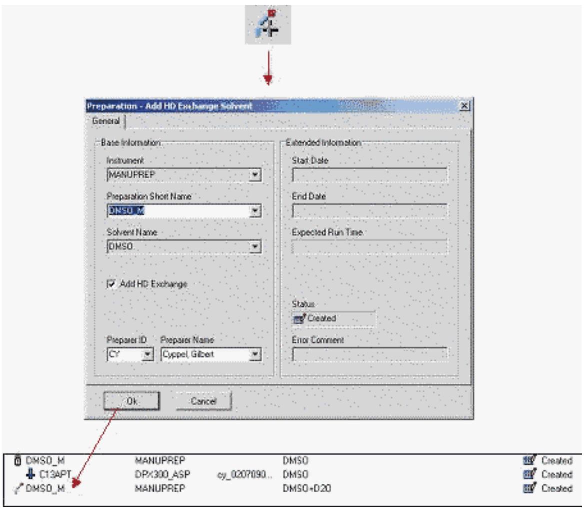
Status: Created

Select the desired instrument and experiment from the respective pull-down menus and change the Analyst blocks if necessary. To commit the new experiment press the OK button. The experiment will then be added and displayed as the next workstep in your sample order. If required, you may enter additional experiments in this same manner.

Adding D20 for Proton Exchange 6.6

If you want to add D2O for a proton exchange experiment to your order, press the Add Proton Exchange button located in the Sample Order Details window. A small Preparation Setup window will appear, allowing you to add the D2O by placing a check in the Add D2O box. Pressing the OK button will return you to the Sample Order Details window, while simultaneously adding the D2O workstep (a workstep with D2O added is shown in the following figure).

Figure 6.9. Add D2O for a Proton Exchange Experiment



Preparation - Add HD Exchange Solvent

Instrument: MANUPREP
Preparation Short Name: DMSO_M
Solvent Name: DMSO
☑ Add HD Exchange
Preparer ID: CY
Preparer Name: Cyppel, Gilbert
Status: Created

DMSO_M	MANUPREP		DMSO	Created
C13APT	DPX300_ASP	cy_0207090...	DMSO	Created
DMSO_M	MANUPREP		DMSO+D20	Created

Add the associated proton experiment as described above (see Adding Experiments) or use the standard Window’s copying procedure to copy an existing proton experiment.

Copy an Existing Experiment 6.7

To copy an existing experiment:

- Press and hold down the Control key on your keyboard.
- Select the gray area to the left of the existing proton experiment with your mouse, and drag the experiment into the gray area under the new preparation.
- Release the mouse button and Control key. The experiment should now be copied under the new preparation. The following figure is a demonstration of this process:

Figure 6.10. Copying an Existing Experiment

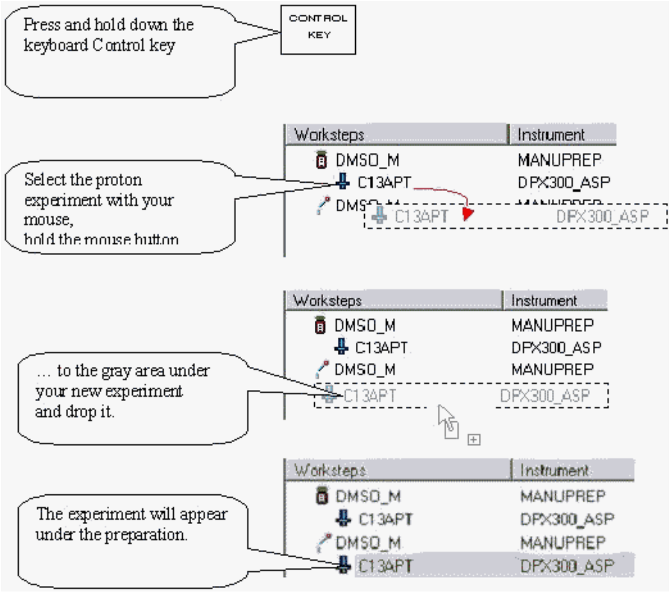
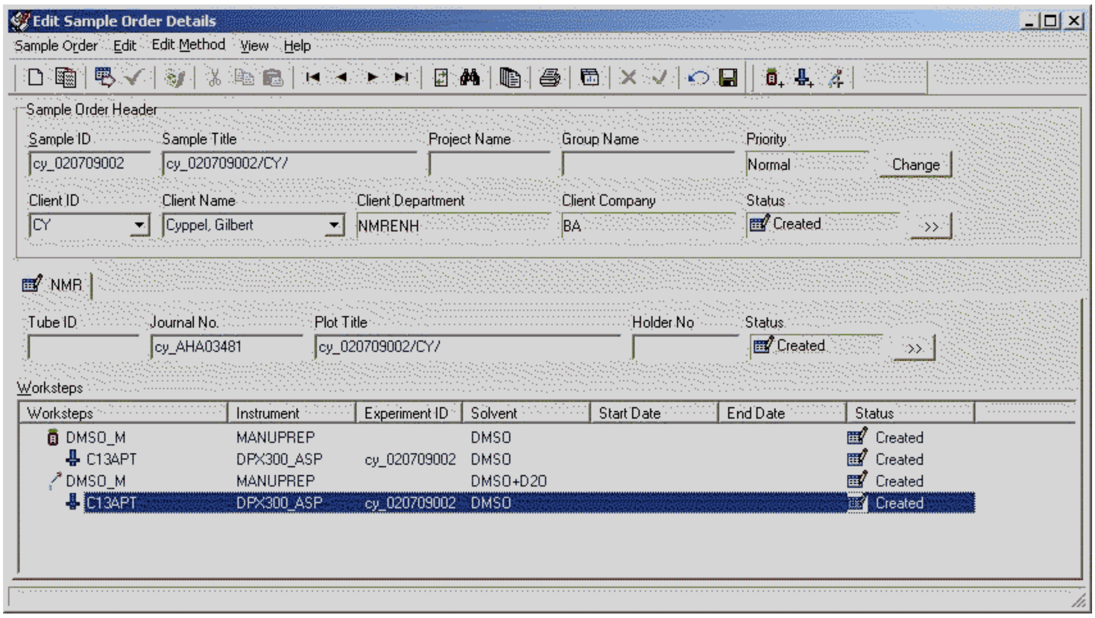

Press and hold down the keyboard Control key
CONTROL KEY
Select the proton experiment with your mouse, hold the mouse button
... to the gray area under your new experiment and drop it.
The experiment will appear under the preparation.
Worksteps
Instrument
DMSO_M
MANUPREP
C13APT
DPX300_ASP

Figure 6.11. A Sample Order Created Using the Copy Function



Sample Order Header

Sample ID: cy_020709002
Sample Title: cy_020709002/CY/
Project Name:
Group Name:
Priority: Normal
Client ID: CY
Client Name: Cyppel, Gilbert
Client Department: NMRENH
Client Company: BA
Status: Created

NMR

Tube ID:
Journal No.: cy_AHA03481
Plot Title: cy_020709002/CY/
Holder No:
Status: Created

Worksteps	Instrument	Experiment ID	Solvent	Start Date	End Date	Status
DMSO_M	MANUPREP		DMSO			Created
C13APT	DPX300_ASP	cy_020709002	DMSO			Created
DMSO_M	MANUPREP		DMSO+D20			Created
C13APT	DPX300_ASP	cy_020709002	DMSO			Created

Starting a Preparation and Measurement 6.8

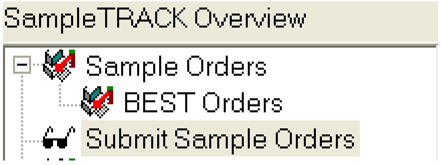
There are two methods available for starting the preparation and/or measurement:

- Standard Method
- Manual Method in the Sample Order Detail Window

Standard Method 6.8.1

The standard method used to start the preparation and measurement is to use the Submit/Verify Sample Orders Tool located in the SampleTrack Overview window.

Figure 6.12. The Submit Window



With this tool all external LIMS imported or manually generated sample orders are viewed and submitted for measurement.

You can submit the sample orders individually with the submit button, or all together by pressing the Select All button (CTRL A) and the Submit button.

The relevant orders for the instrument will then be generated for all submitted sample orders.

Note: Delayed experiments will not be generated until the start time has elapsed.

Manual Submit in the Sample Order Details Window 6.8.2

As an alternative method it is also possible to start an individual order generation by using the **Submit Sample Order** button in the Sample Order Details window.

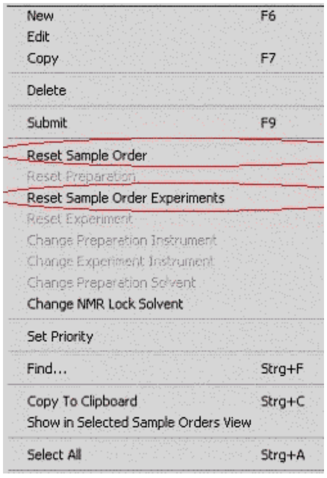
This method is effective only when you have a limited amount of orders.

Rerunning a Faulty or Finished Experiment 6.9

Mark the order and select one of the following options:

- Reset complete Sample Order
- Reset Sample Order Experiments

Figure 6.13. Rerun an Experiment

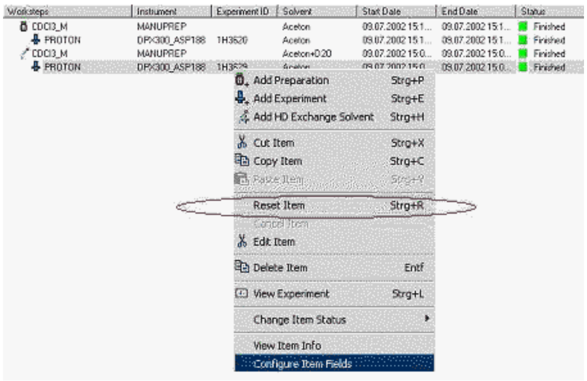


Resetting a distinguished experiment or a preparation is possible in the Sample Order Details window. Select the desired faulty or finished experiment or preparation by marking it, and use the right mouse button to select **Reset Item** (Ctrl R). This will set the status to **Created**.

Now resubmit the order.

In the case, where the whole order with preparation should be restarted, use **Reset Sample Order.** Submit the order to start the experiment.

Reset Item to Rerun the Complete Order



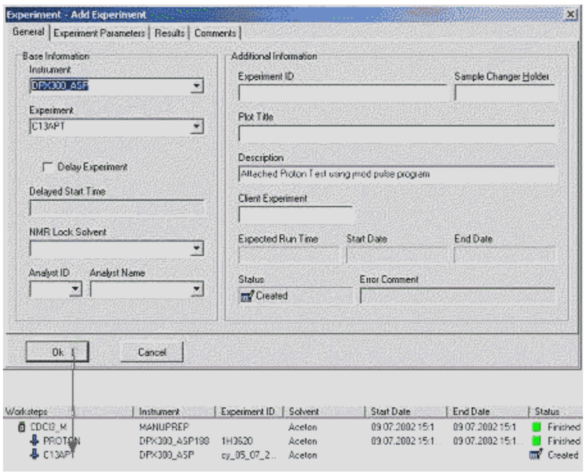
Worksteps	Instrument	Experiment ID	Solvent	Start Date	End Date	Status
CDCl3_M	MANUPREP		Aceton	09.07.2002 15:1...	09.07.2002 15:1...	🟩 Finished
PROTON	DPX300_ASP188	1H3620	Aceton	09.07.2002 15:1...	09.07.2002 15:1...	🟩 Finished
CDCl3_M	MANUPREP		Aceton+D20	09.07.2002 15:0...	09.07.2002 15:0...	🟩 Finished
PROTON	DPX300_ASP188	[illegible]	Aceton	09.07.2002 15:0	09.07.2002 15:0...	🟩 Finished

Adding an Experiment to a Finished Sample Order 6.10

At times it may be desirable to add an additional experiment to a finished sample order. To do so please follow the instructions below.

- Move to the Sample Order Details window of the relevant sample order by double-clicking on the order.
- Click once on the last experiment of the preparation in the Worksteps block and press the Add Experiment button. The Insert a new Experiment window will appear.
- Select the desired Instrument and Experiment data and update the Analyst blocks if required.
- When the parameters are acceptable confirm them by pressing the OK button.
- Start the measurement of your new experiment by pressing the Verify/Submit Sample Order button.

Figure 6.14. Adding an Additional Experiment



Instrument: DPX300_ASP

Experiment: C13APT

☐ Delay Experiment

Description: Attached Proton Test using mod pulse program

Status: Created

Worksteps	Instrument	Experiment ID	Solvent	Start Date	End Date	Status
CDCl3_M	MANUPREP		Aceton	09.07.2002 15:1	09.07.2002 15:1	🟩 Finished
PROTON	DPX300_ASP198	1H3620	Aceton	09.07.2002 15:1...	09.07.2002 15:1...	🟩 Finished
C13APT	DPX300_ASP	cy_05_07_2...	Aceton			Created

Filter and Search Tools 6.11

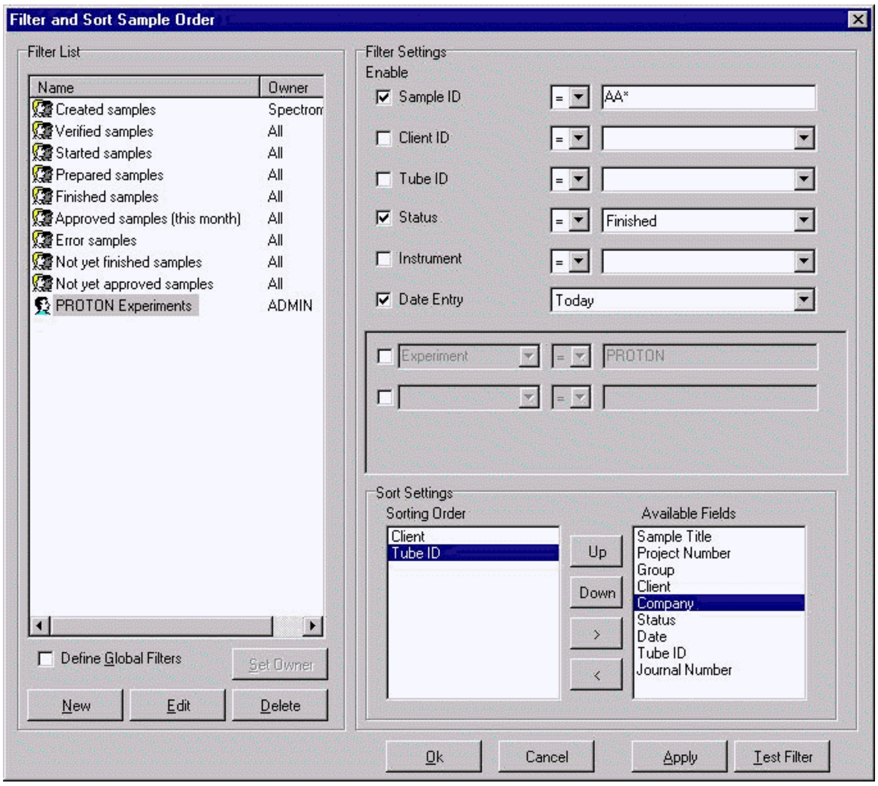
Filter Tools 6.11.1

SampleTrack™ runs in combination with the relational Oracle database, therefore, the displaying all of the stored sample orders is quite inefficient. The use of configurable filters reduces this inefficiency by allowing you to select only the samples that meet your search criteria.

Many of the window views within SampleTrack™ allow the user to define various filters. The user specific filters can be stored with a user defined name and are available after each new log-in. To open the filter definition window, press the button located to the right of the filter bar in the respective window.

A Filter and Sort Sample Order window will appear, which will allow you to define a variety of filter settings, or select an existing filter.

Figure 6.15. Example of a Filter Definition



Filter and Sort Sample Order

Filter List

Name	Owner
Created samples	Spectrom
Verified samples	All
Started samples	All
Prepared samples	All
Finished samples	All
Approved samples (this month)	All
Error samples	All
Not yet finished samples	All
Not yet approved samples	All
PROTON Experiments	ADMIN

☐ Define Global Filters

Filter Settings

Enable		
☑ Sample ID	=	AA*
☐ Client ID	=	
☐ Tube ID	=	
☑ Status	=	Finished
☐ Instrument	=	
☑ Date Entry		Today
☐ Experiment	=	PROTON
☐	=	

Sort Settings

Sorting Order	Available Fields
Client	Sample Title
Tube ID	Project Number
	Group
	Client
	Company
	Status
	Date
	Tube ID
	Journal Number

In the example above a filter with the following functions has been defined:

All sample ID’s begin with **AA**, have a status **Finished** and are sorted in Client ID and Tube ID order.

When creating a new filter you should always use a meaningful name to ease identification at a later time.

Defining these special filters makes working with SampleTrack™ both efficient and easy.

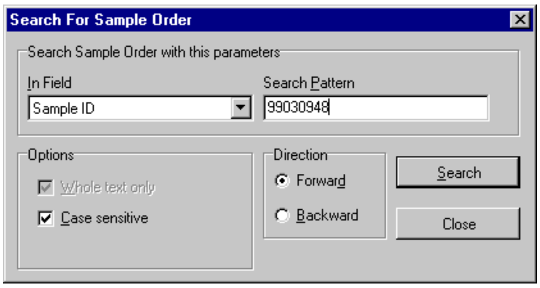
Search Tools

Although working with the filters search function makes SampleTrack™ efficient and easy, it does not eliminate the desirability of a standard search function. To ease searching for a specific Sample ID, Tube ID etc., a standard search function has been implemented in SampleTrack™.

There are two separate search possibilities, one in the Client Tool window, and one in the Sample Order Details window.

The Client Tool window has a Search in View feature that will **search through the current list of data in the display window** for a specific parameter. To perform this search, press the Search in View button located at the top of the Client Tool window.

Figure 6.16. Search in View - Client Tool Window



Search For Sample Order

Search Sample Order with this parameters

In Field: Sample ID

Search Pattern: 99030948

Options

☑ Whole text only

☑ Case sensitive

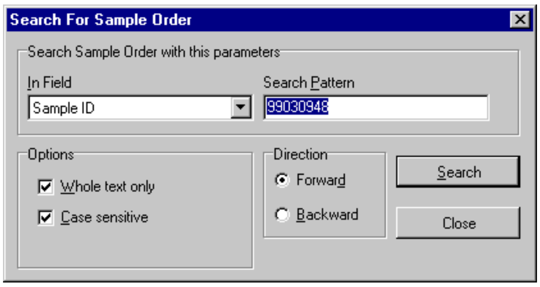
Direction

● Forward

○ Backward

The Sample Order Details window has a Search in DB feature that will **search through the Oracle® database** for a specific parameter that you specify. To perform this search, press the Search in DB button located at the top of the Sample Order Details window.

Figure 6.17. Search in DB - Sample Order Details Window



Search For Sample Order

Search Sample Order with this parameters

In Field: Sample ID

Search Pattern: 99030948

Options

☑ Whole text only

☑ Case sensitive

Direction

● Forward

○ Backward

In both cases select the relevant search field from a list of values in the In Field pull-down menu and enter your search parameter in the Search Pattern field. If your search is to be case sensitive, check the Case Sensitive box. You can also indicate whether you want to search in ascending or descending order by selecting Forward or Backward in the Direction box.

Press Search to begin the search operation, or close to cancel and exit the window.

If the search program reaches the end of the list (when you are searching while in the Client Tool) without finding your search parameter, you will be prompted whether you want to restart from the beginning. This is significant if you have started your search in the middle of the list. In this case, press Yes to continue, or No to end the current search.

Attention! The search function corresponds directly with your selected filters. Therefore, you will not find information outside of your filtered data.

Interaction with Analytical Applications

7

Interaction with TOPSPIN®

7.1

SampleTrack™ allows you to directly call TOPSPIN® with your associated experiment data set. This results in easy verification of measurement results and structure elucidation.

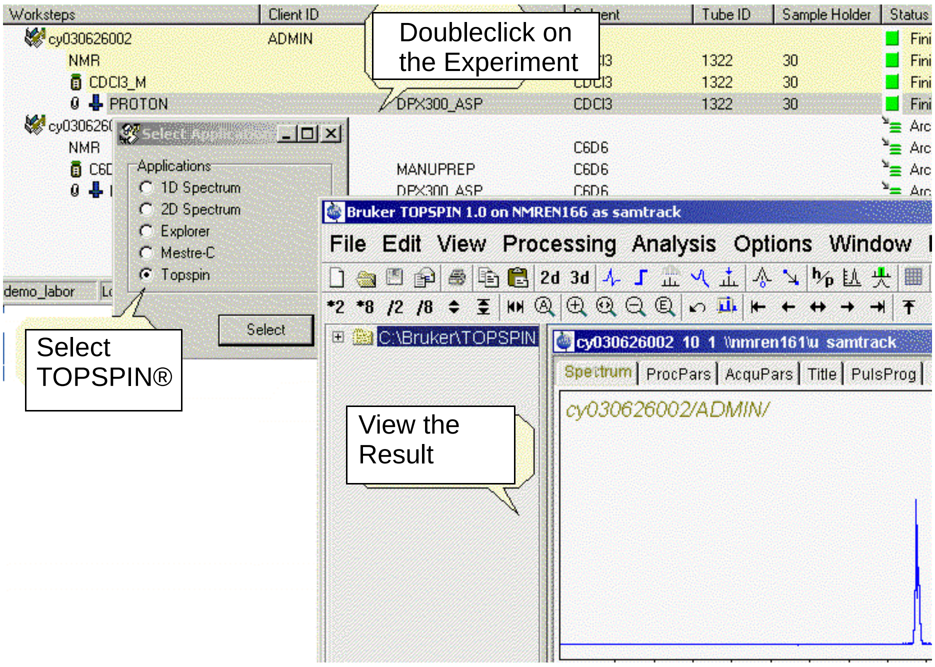
Figure 7.1. The Paperclip Icon

The paperclip icon to the left of the experiment symbol shows existing experiment paths.

Doubleclick an experiment marked with the paperclip icon. After selecting TOPSPIN® SampleTrack™ transfers the information about the location of the data set to the program. TOPSPIN® then converts the data and displays it on the screen.

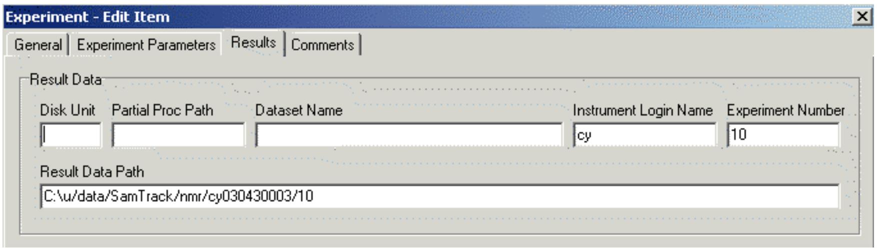
With the View next Experiment button, the program automatically switches to the next experiment and passes the associated data to TOPSPIN®.

Figure 7.2. *Interaction with TOPSPIN®*


Doubleclick on the Experiment
Select TOPSPIN®
View the Result
Select Application
Applications
1D Spectrum
2D Spectrum
Explorer
Mestre-C
Topspin
Select
Bruker TOPSPIN 1.0 on NMREN166 as samtrack
File Edit View Processing Analysis Options Window
C:\Bruker\TOPSPIN
cy030626002 10 1 \\nmren161\u samtrack
Spectrum ProcPars AcquPars Title PulsProg
cy030626002/ADMIN/
Worksteps
Client ID
Tube ID
Sample Holder
Status

The result data path is stored in the database and can be seen in the experiment detail view.

Figure 7.3. The Results Data Path



Disk Unit:
Partial Proc Path:
Dataset Name:
Instrument Login Name: cy
Experiment Number: 10
Result Data Path: C:\u/data/SamTrack/nmr/cy030430003/10

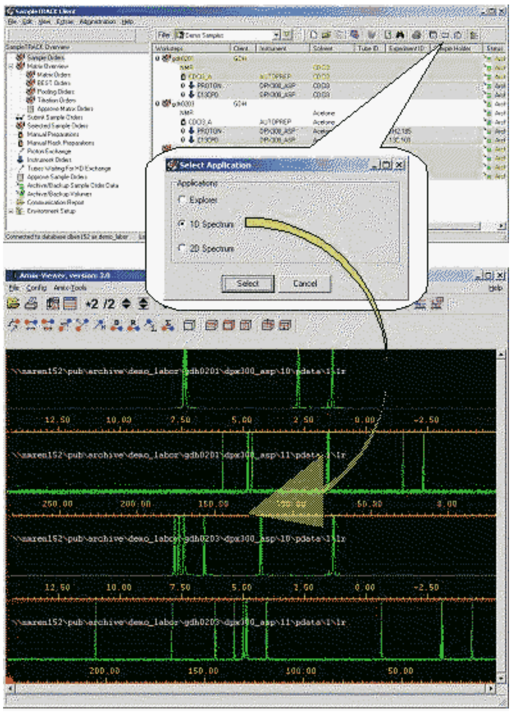
Interaction with AMIX™ 7.2

SampleTrack™ allows you to directly call AMIX™ with your associated experiment data set. This results in easy verification of measurement results and structure elucidation.

The paperclip icon to the left of the experiment symbol shows existing experiment paths.

📎

Figure 7.4. Interaction with AMIX™


Select Application
Applications
Explorer
1D Spectrum
2D Spectrum
Select
Cancel
Amix-Viewer, version: 3.0
File
Config
Amix-Tools
\\maren152\pub\archive\demo_labor\gdh0201\dpx300_asp\10\pdata\1\1r
\\maren152\pub\archive\demo_labor\gdh0201\dpx300_asp\11\pdata\1\1r
\\maren152\pub\archive\demo_labor\gdh0203\dpx300_asp\10\pdata\1\1r
\\maren152\pub\archive\demo_labor\gdh0203\dpx300_asp\11\pdata\1\1r
12.50
10.00
7.50
5.00
2.50
0.00
-2.50
250.00
200.00
150.00
100.00
50.00
0.00

Applications: ● 1D Spectrum

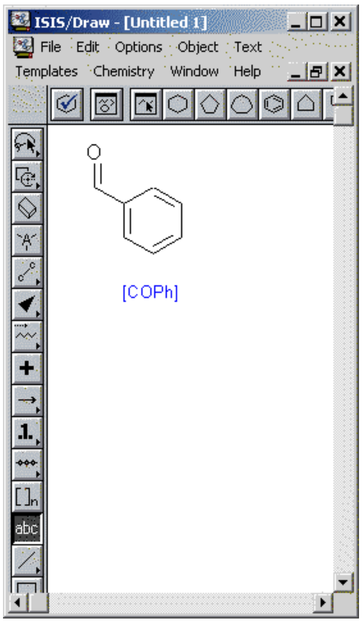
Interaction with Structure Editors 7.3

SampleTrack™ also allows you to call a structure editor e.g. MDL® ISIS/Draw™ where you can enter the expected chemical structure results.

This feature is also activated in the Sample Order Details window by pressing the Documents button, and selecting Structure. The Structure Editor program will then be opened and the sample structure can be viewed. Usually the structure is entered when the sample order is created. The saved file will be linked with the sample order. The file name could be for example the laboratory journal number or the sample order number or a project number.

If desired a template file with customized settings can be opened as default.

Figure 7.5. MDL® ISIS/Draw™ Template



Interaction with other Windows® Applications 7.4

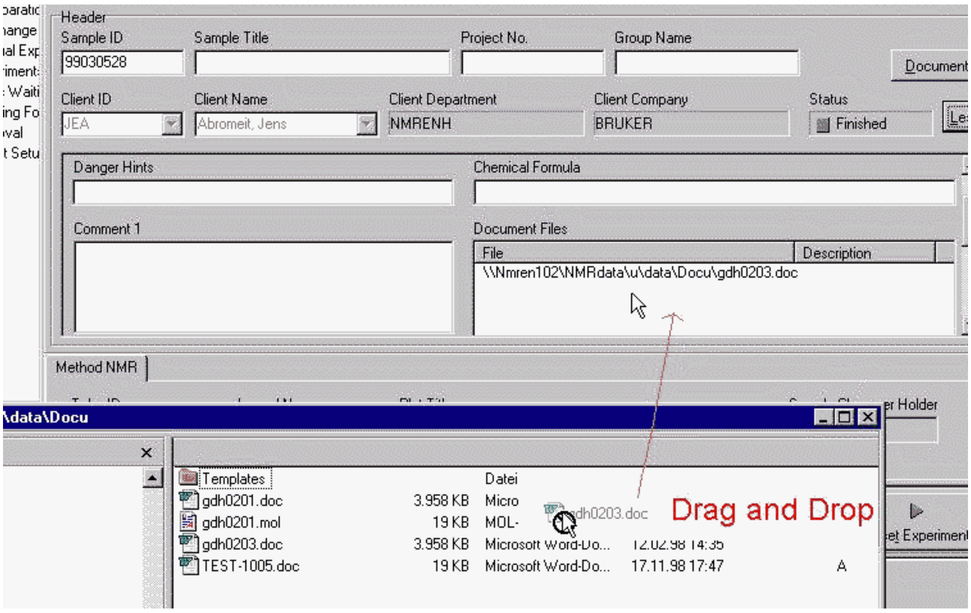
SampleTrack™ allows you to link to other Microsoft Windows® applications (e.g. for reports) directly from the Sample Order Details window.

To create a new UNC (Universal Naming Convention) formatted link to an existing Microsoft Word® document, for example, open the Sample Order Details window and click on the **More** button.

Figure 7.6. The More Button.

This will expand the viewing options to include a Document Files box. Open the Windows® Explorer, and drag the desired file to the Document Files box, and drop it in the box. This will create a UNC format link to the desired file.

Figure 7.7. Creating a New UNC Formatted Link to a Document File



Sample ID: 99030528

Client ID: JEA
Client Name: Abromeit, Jens
Client Department: NMRENH
Client Company: BRUKER
Status: Finished

Document Files

File	Description
\\Nmren102\NMRdata\u\data\Docu\gdh0203.doc	

\data\Docu

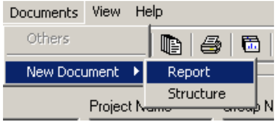
		Datei		
Templates				
gdh0201.doc	3.958 KB	Micro		
gdh0201.mol	19 KB	MOL-		
gdh0203.doc	3.958 KB	Microsoft Word-Do...	12.02.98 14:35	
TEST-1005.doc	19 KB	Microsoft Word-Do...	17.11.98 17:47	A

Once a new UNC formatted link has been created you must only double-click on this link to open e.g. Microsoft Word® to view the file.

Creating a New Report Within the Details Window *7.5*

It is also possible to create a new report within the Sample Order Details window. To create a new report press the Documents button, then select New Document - Report as shown in the following figure.

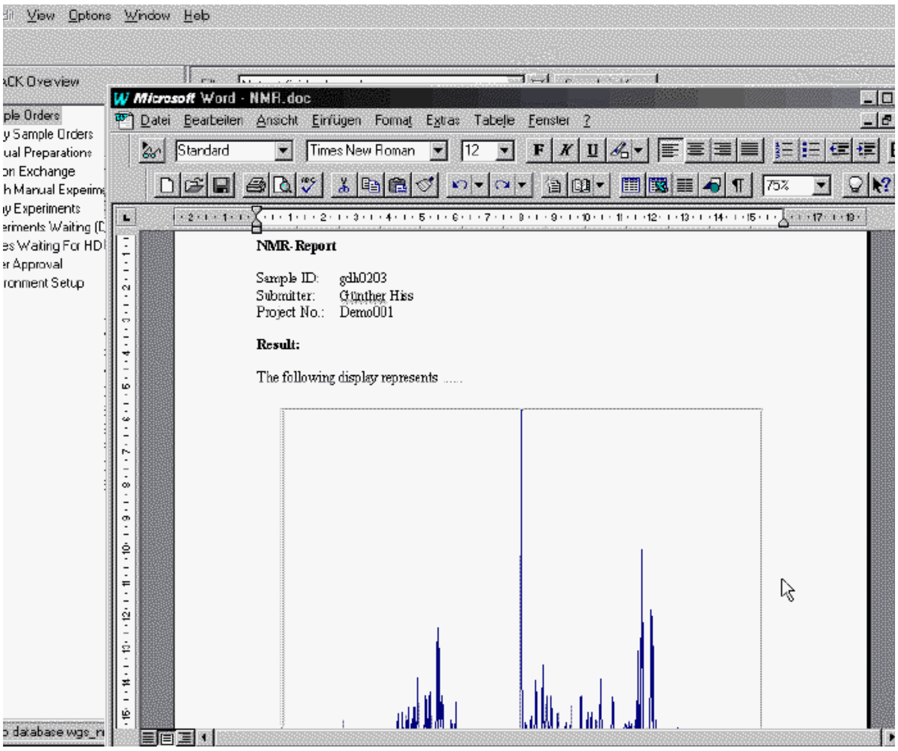
Figure 7.8. Creating a New Report



This will open a report template file in your default word processor (e.g. Microsoft® Word). The file will automatically be saved as the pre-selected destination file.

This will work only if you have set the appropriate parameters in the Options - General Settings - Applications - Report menu in the SampleTrack™ Client window (See next chapter).

Figure 7.9. An Example of a Report



NMR-Report

Sample ID: gdh0203
Submitter: Günther Hiss
Project No.: Demo001

Result:

The following display represents .....

Application Management 7.6

The definition of all applications in SampleTrack™ can be found using the menu **Administration - Application management.**

In the Application Management window, on the left side, all existing applications are displayed. To add or copy an application, use the right mouse button. On the right side of the window are the options **mixed, global** and **local**. These options allow you to display various kind of entries:

Mixed is a view of the entries in the global and local window.

Global entries are saved in the SampleTrack™ database. They consist of data used by the most or all the users.

For example, the program executable path for 90% of the SampleTrack™ users in one company could be:

C:\Programme\Microsoft Office\Office\WINWORD.EXE.

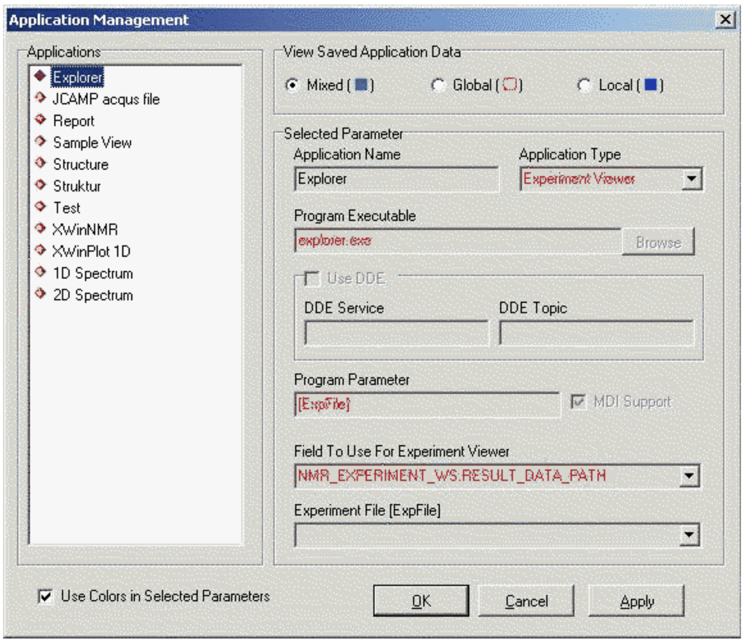
And the rest of the users could have a path like

C:\Program folders\Microsoft Office\Office\WINWORD.EXE.

In this example local entry is written, which is different from the global entries. The program reads the local entry first, and then the global entry.

If an additional program is used only by a few people: this program must be defined in the local viewer. These definings will be saved in the local registry of the PC.

Figure 7.10. Administration - Application Management



View Saved Application Data: ● Mixed (■) ○ Global (☐) ○ Local (■)

Application Name: Explorer

Application Type: Experiment Viewer

Program Executable: explorer.exe

☐ Use DDE

Program Parameter: [ExpFile]

☑ MDI Support

Field To Use For Experiment Viewer: NMR_EXPERIMENT_WS.RESULT_DATA_PATH

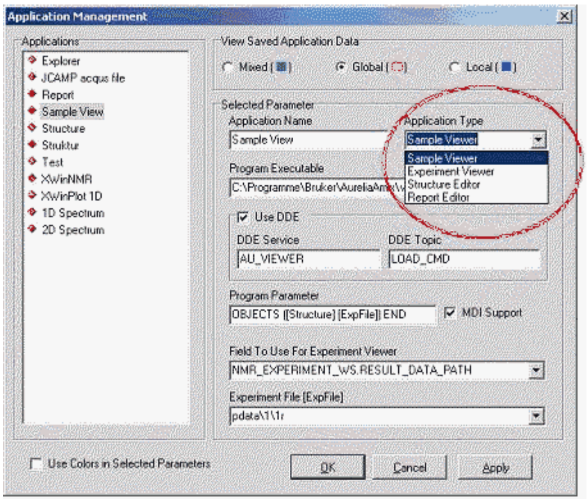
Experiment File [ExpFile]:

☑ Use Colors in Selected Parameters

Application Type 7.6.1

The Application type decides in which environment within SampleTrack™ an application may be started.

Figure 7.11. Defining the Application Type



View Saved Application Data: ○ Mixed (■) ● Global (☐) ○ Local (■)

Application Name: Sample View

Application Type: Sample Viewer

Program Executable: C:\Programme\Bruker\AureliaAm

☑ Use DDE

DDE Service: AU_VIEWER

DDE Topic: LOAD_CMD

Program Parameter: OBJECTS ([Structure] [ExpFile]) END

☑ MDI Support

Field To Use For Experiment Viewer: NMR_EXPERIMENT_WS.RESULT_DATA_PATH

Experiment File [ExpFile]: pdata\1\1r

☐ Use Colors in Selected Parameters

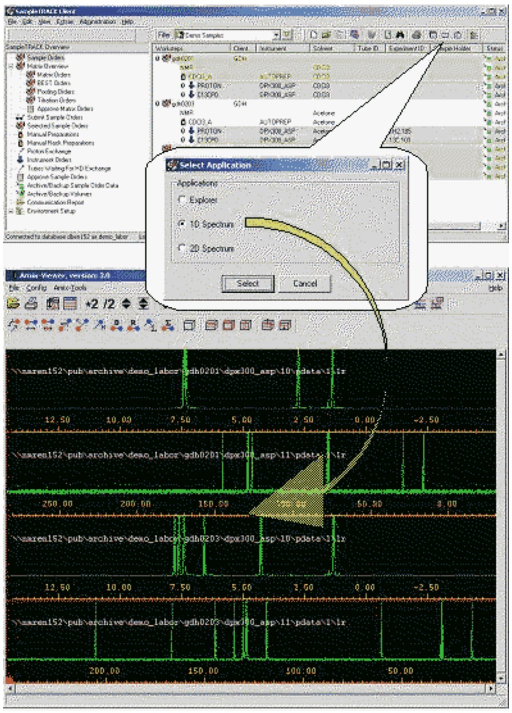
- Sample Viewer (one or more experiments in an order)
- Experiment Viewer (one or more experiments with different orders)
- Structure Editor (IMDL® *ISIS/Draw*™/MESTRE-C™ or others)
- Report Editor (Word®/Excel®)

Selecting Applications in the Sample Order Window 7.6.2

In the **Sample Order View** the **Application Selection** window is called by simple double clicking the experiment (Experiments with the papeclip icon only!).

You can also mark one or more experiments in the **sample orders view** window and click the **’view the selected experiments’** button.

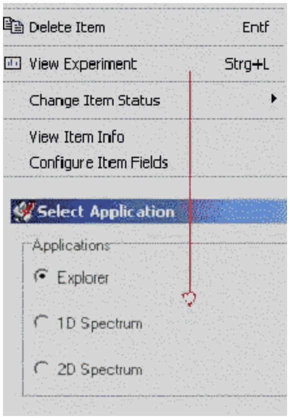
Figure 7.12. Example 1: Select Application



Selecting Applications in the Detail Window 7.6.3

The Applications defined as **’Experiment Viewer’** is selectable in the **order detail** window pressing the right mouse button as shown in the next figure.

Figure 7.13. Example 2: Select Application



EasyDialog

8

Introduction to EasyDialog 8.1

EasyDialog is a program that provides administrator-definable forms that allow an open access user to quickly and easily add a sample order to SampleTrack™. EasyDialog is ideal for a user who needs to quickly add a routine sample order, or for an inexperienced user to easily begin productivity.

EasyDialog lacks the full features obtained by using the Add Sample Order in the client window, however, provides a productivity-enhancing feature for routine orders.

The administrator can configure EasyDialog for individual or groups, based on their specific requirements.

Opening EasyDialog 8.2

To open the EasyDialog window press the Windows® Start button and select SampleTrack™ - EasyDialog.

Figure 8.1. EasyDialog Icon

After a moment, a login window will appear, prompting you to login to EasyDialog.

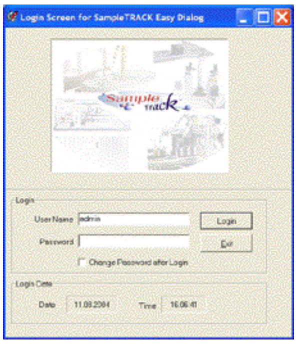
EasyDialog Login Window 8.3

After you enter your login name and password, press the Login button to finish the start-up process. The EasyDialog Window will appear, similar to the one shown below. Remember that your specific dialog window may vary depending on how the administrator has configured it. If you have questions on specific features of your EasyDialog window, check with your administrator.

Note: If you have administrator privileges, you can also start EasyDialog by selecting File - Open EasyDialog from the SampleTrack™ Client Tool. Refer to the EasyDialog Configuration help for details

"Opening the EasyDialog Configuration Window" on page 123.

Figure 8.2. EasyDialog Login


Login Screen for SampleTRACK Easy Dialog
Sample "E" track
Login
Login
Exit
☐ Change Password after Login
Login Data

User Name: admin

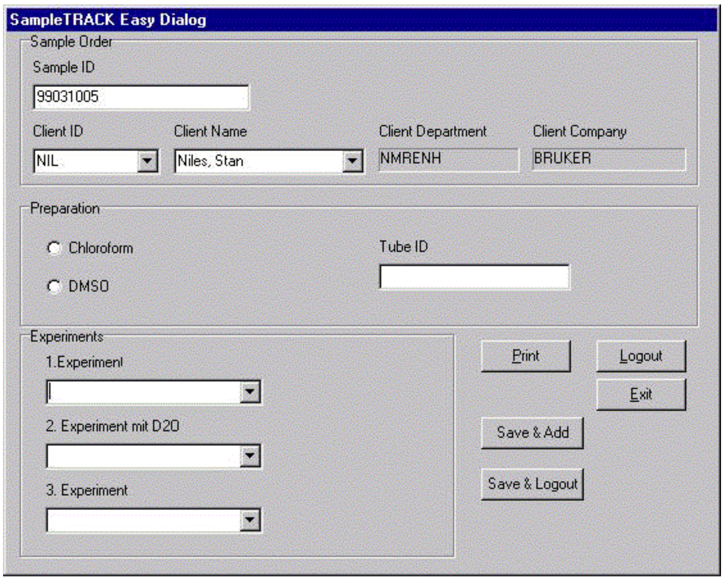
Password:

Date: 11.08.2004

Time: 16:06:41

The EasyDialog Window 8.4

Figure 8.3. EasyDialog Example



Sample ID: 99031005

Client ID: NIL

Client Name: Niles, Stan

Client Department: NMRENH

Client Company: BRUKER

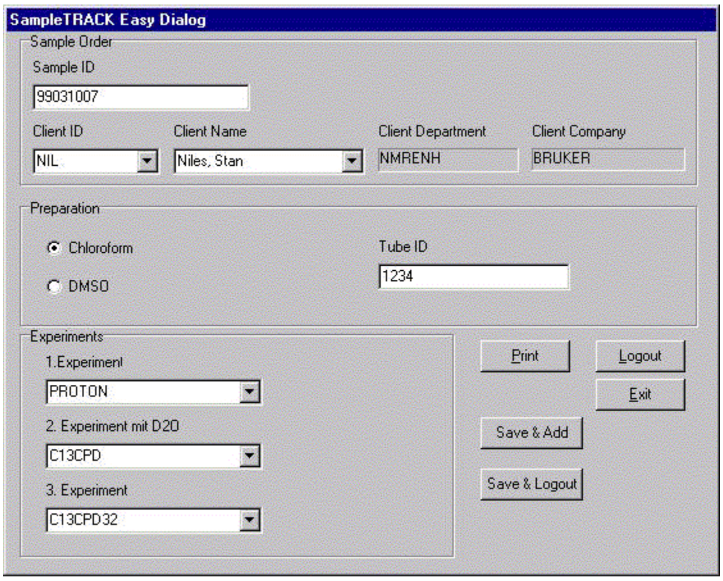
Tube ID:

In the EasyDialog example above the sample order information is automatically loaded when the window is opened (this is an administrator-configurable option). To add a sample order you must only select or enter the required preparation and experiment parameters and press one of the corresponding buttons.

Entering Data in the EasyDialog Window 8.5

When you enter the data as shown in the figure below, and then press **Save & Add**, the new sample order will be automatically added to the SampleTrack™ database. A confirmation message will be displayed when this process is complete.

Figure 8.4. Entering Data with EasyDialog

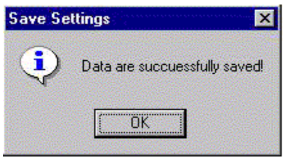


Sample ID: 99031007
Client ID: NIL
Client Name: Niles, Stan
Client Department: NMRENH
Client Company: BRUKER
● Chloroform
○ DMSO
Tube ID: 1234
1.Experiment: PROTON
2. Experiment mit D2O: C13CPD
3. Experiment: C13CPD32

EasyDialog Confirmation Message 8.6

The EasyDialog window will remain open after the confirmation of a data entry so that you can add additional sample orders. In this example if you wanted to add only the one sample order you could press Save & Logout, which would add the order to the database, but would then exit EasyDialog.

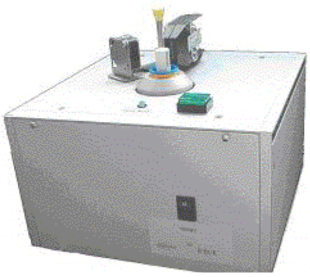
Figure 8.5. EasyDialog Confirmation Message



Data are succuessfully saved!

The above example is just one of many different features that an administrator can add to EasyDialog. EasyDialog can be configured for your own unique group or individual laboratory requirements.The EasyDialog field **tube ID** can be automatically filled out by the barcode reader from B-BCEThe tube ID is inserted automatically by pressing the green button on the B-BCE.

Figure 8.6. Automatic Reading of the Barcode Tube ID



SampleTrack™ Web Client

9

WEB Client - Introduction 9.1

The **SampleTrack Web Client** allows connection to the SampleTrack database with a standard HTML browser from any PC, that has connection to the Internet or company Intranet – without additional installation of the SampleTrack Client software.

Its functionality does not cover the whole SampleTrack spectrum but is sufficient for most standard measurements. All information for a sample order can be queried and with the **EasyWeb Dialog** tool orders can be initiated the same way as EasyDialog does.

Within the **SampleTrack Web Client** services are available for structure and spectra viewing or as a quick evaluation tool. For a more intensive evaluation, an application wizard is available, that can call TOPSPIN® , AMIX™ or other used applications directly.

SampleTrack Web Client is optimized for Microsoft® Internet Explorer version 5.0 or higher, but is compatible with common browsers like Netscape®, Mozilla™ or Opera®.

Although Java simplifies the HTML handling, the SampleTrack Web Client does not use any Java applets.

All user and group profiles, group filters and views that were previously defined with the SampleTrack administration tool are integrated within the web tool. An additional configuration is not necessary.

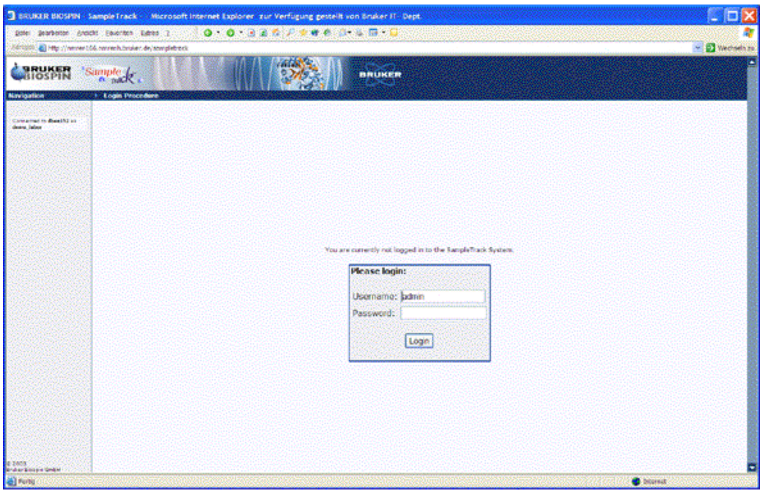
All data sent through the Web can be secured by a secure connection with SSL.

For the SampleTrack Web Client installation see ***"Installation" on page 225***

Viewing Sample Orders 9.2

To view sample orders, login into the **SampleTrack Web Client** using the SampleTrack user name and password:

Figure 9.1. SampleTrack Web Client Login


BRUKER BIOSPIN - SampleTrack - Microsoft Internet Explorer zur Verfügung gestellt von Bruker IT- Dept.
BRUKER BIOSPIN
SampleTrack
BRUKER
Navigation
Login Procedure
Login

You are currently not logged in to the SampleTrack System.

Please login:

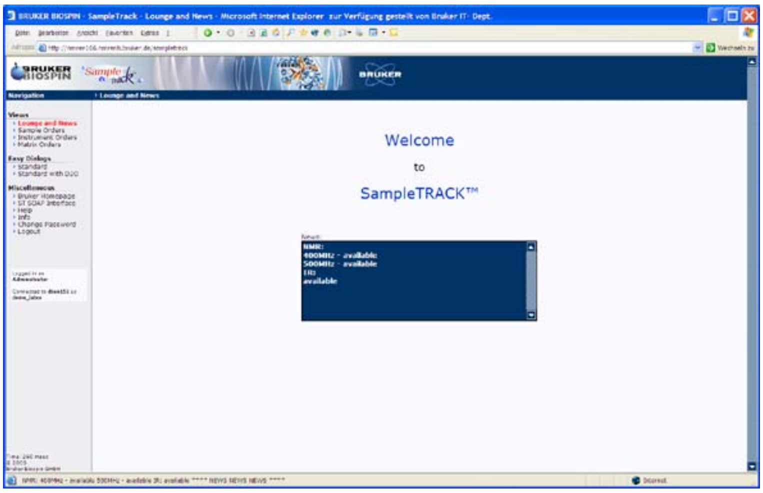
Username: admin

Password:

In the left frame the following views are available:

- Sample Orders: Complete orders within the SampleTrack system.
- Instrument orders: Order information related to an instrument
- Matrix orders: Order information about matrix orders like BEST
- EasyWeb Dialog

Figure 9.2. Navigation Board



Welcome

to

SampleTRACK™

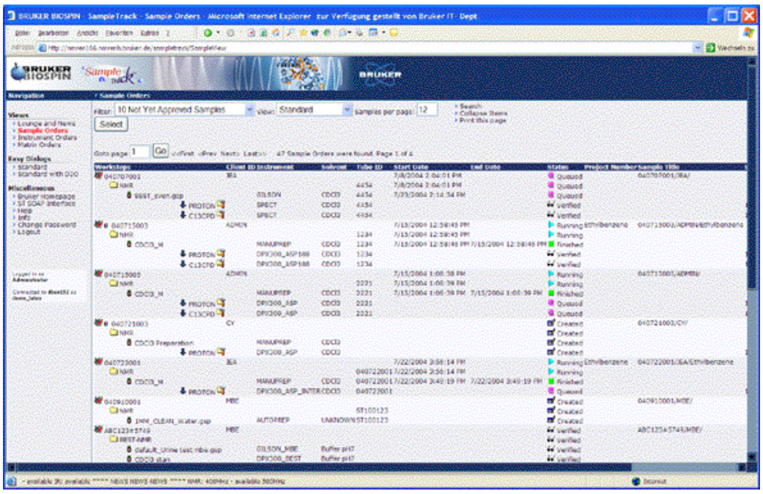
NMR:
400MHz - available
500MHz - available
IR:
available

Sample Orders – View *9.2.1*

The **Sample Order View** lets you track the orders and view their results. You can select your favourite view by selecting the various filters in the upper window. These individually customizable selections let you view the fields that are of interest. The other selection window, which also has customizable filters, lets you select only the records that are of interest – personal orders, orders of a department or orders with a predifined status. Working with these filters and views are identical as those found in the SampleTrack client.

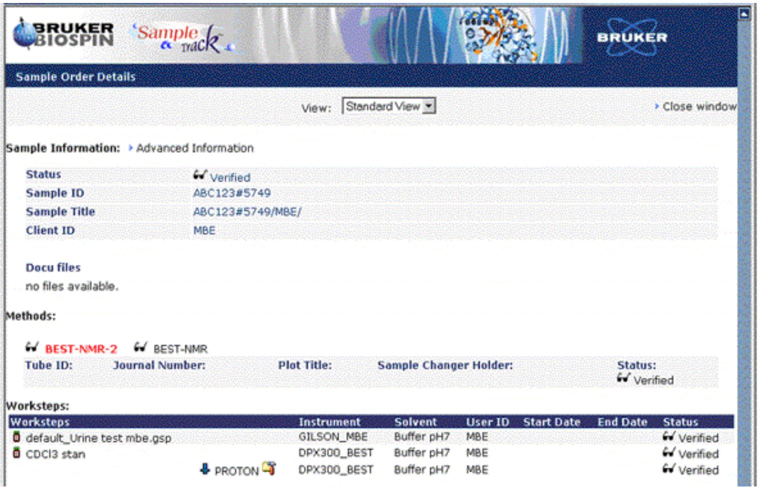
The number of records that can be displayed in one window can be entered in the upper window. Navigation through the pages is possible using the links „First, Prev, Next, Last“. A link “Print this page” navigates to a printer friendly view.

Figure 9.3. Sample Orders - View



The worksteps are presented in a tree view, as is within the SampleTrack client. By clicking on the sample ID, the method, the preparation or the experiment the program navigates to a window with more detailed information. In the **Detailed Sample Order** window information can be found on the complete order, e.g. methods, attached documents or comments.

Figure 9.4. Complete Order



Sample Order Details

View: Standard View

Close window

Sample Information: Advanced Information

Status	Verified
Sample ID	ABC123#5749
Sample Title	ABC123#5749/MBE/
Client ID	MBE

Docu files

no files available.

Methods:

BEST-NMR-2 BEST-NMR

Tube ID:	Journal Number:	Plot Title:	Sample Changer Holder:	Status:
				Verified

Worksteps:

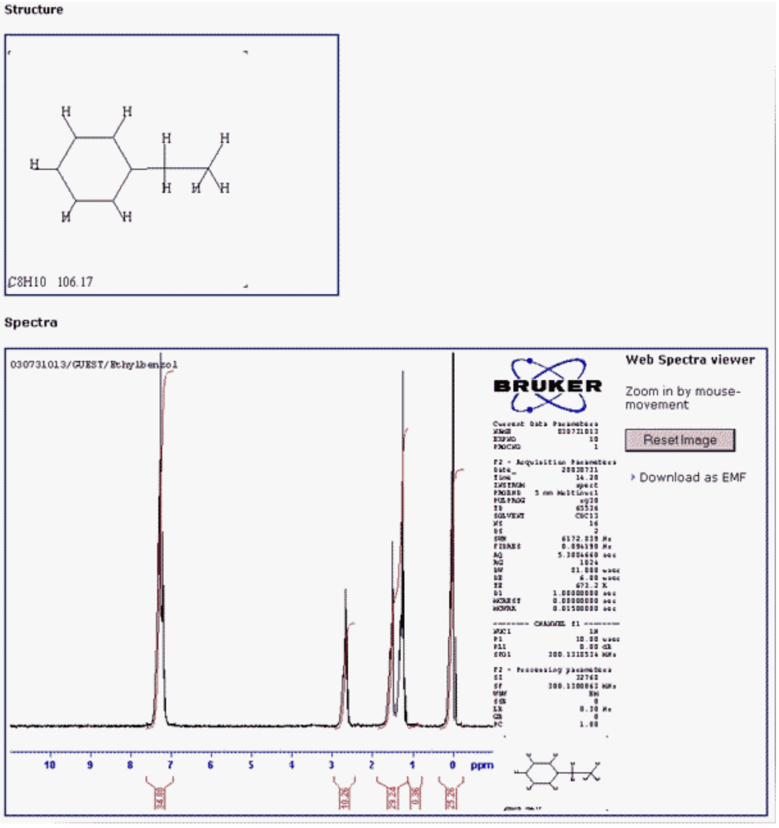
Worksteps	Instrument	Solvent	User ID	Start Date	End Date	Status
default_Urine test mbe.gsp	GILSON_MBE	Buffer pH7	MBE			Verified
CDCl3 stan	DPX300_BEST	Buffer pH7	MBE			Verified
PROTON	DPX300_BEST	Buffer pH7	MBE			Verified

Structure and Web Spectra Viewer *9.2.2*

The SampleTrack Web client provides structure and spectra viewing capabilities, including zooming in and out. Zoom In – Zoom Out

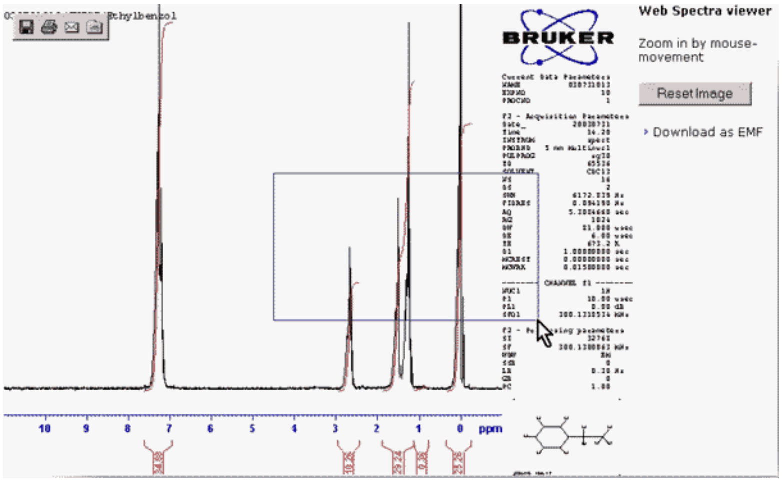
To view distinct areas of spectra click at the starting point, choose the area to be zoomed in (without clicking), and click to confirm. The area selected is also shown in the printer friendly view.

Figure 9.5. Web - Structure and Spectra Viewer



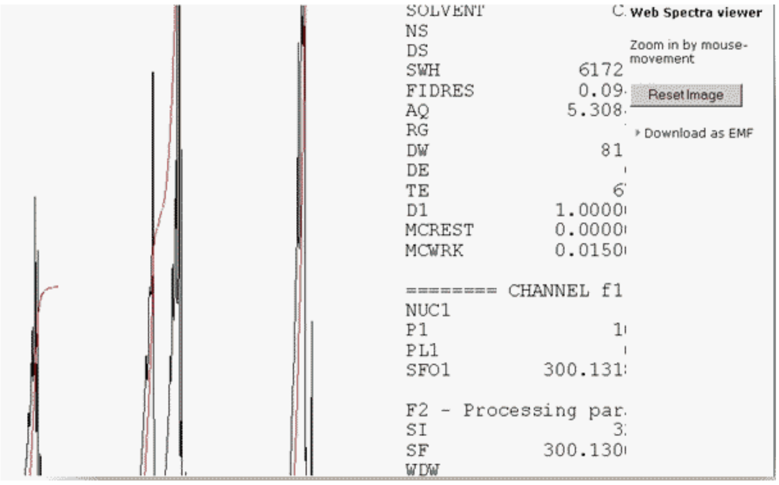
Click the upper left corner once and afterwards click the lower right corner to zoom in.

Figure 9.6. Web - Structure and Spectra Viewer, Zooming In



To review the original size just click the **Reset Image** button

Figure 9.7. Web - Structure and Spectra Viewer, Reset Image



```
SOLVENT            C
NS
DS
SWH             6172
FIDRES          0.09
AQ              5.308
RG
DW                81
DE
TE                 6
D1            1.0000
MCREST        0.0000
MCWRK         0.0150

======== CHANNEL f1
NUC1
P1                 1
PL1
SFO1         300.131

F2 - Processing par
SI                 3
SF           300.130
WDW
```

After finishing an experiment, the **Experiment Detail** window shows the spectra results, when XWIN-PLOT™ has been triggered to generate the results as emf-file.

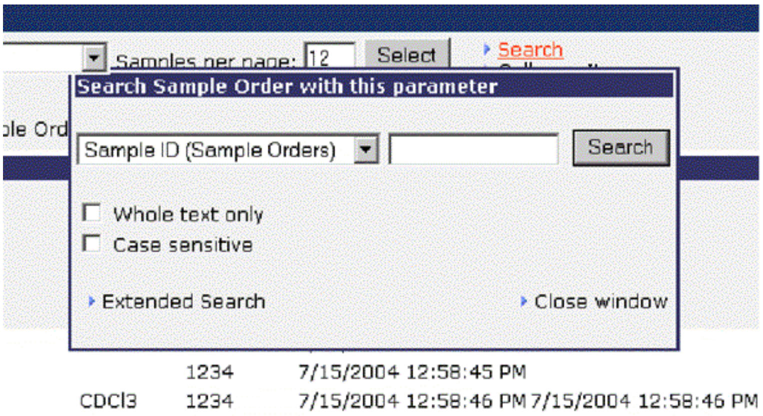
Search 9.2.3

The link „Search“ provides the possibility of performing a manual search, e.g. for a sample ID. Select the kind of field information to search, such as sample ID, status or a date and the search criteria.

When „Whole text only“ is checked, the program searches for an exact match.

When „Whole text only“ is unchecked, the program looks for patterns that include the entered words, e.g. “BCD” finds “ABCD123”.

Figure 9.8. Search



Search Sample Order with this parameter

Sample ID (Sample Orders)

☐ Whole text only

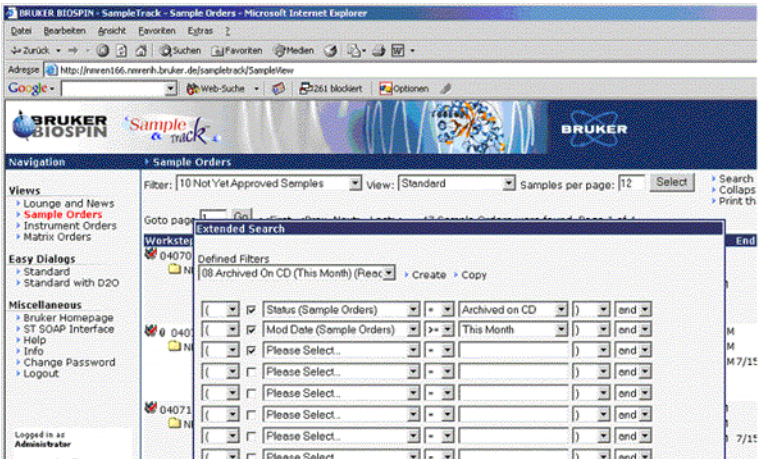
☐ Case sensitive

Samples per page: 12
Select
Search
Search
Extended Search
Close window
1234 7/15/2004 12:58:45 PM
CDCl3 1234 7/15/2004 12:58:46 PM 7/15/2004 12:58:46 PM

Extended Search 9.2.4

With the link „Extended Search“ the Web module (like SampleTrack client) provides more complexe queries over several database fields. Remember, that you can only find records within your predefined datapool, that were defined as your group filter. Changes here can only be made by the administrator in the SampleTrack client.

Figure 9.9. Extended Search



Extended Search

Defined Filters: 08 Archived On CD (This Month) (Reac

(☑ Status (Sample Orders) = Archived on CD) and

(☑ Mod Date (Sample Orders) >= This Month) and

(☑ Please Select.. =) and

(☐ Please Select.. =) and

(☐ Please Select.. =) and

(☐ Please Select.. =) and

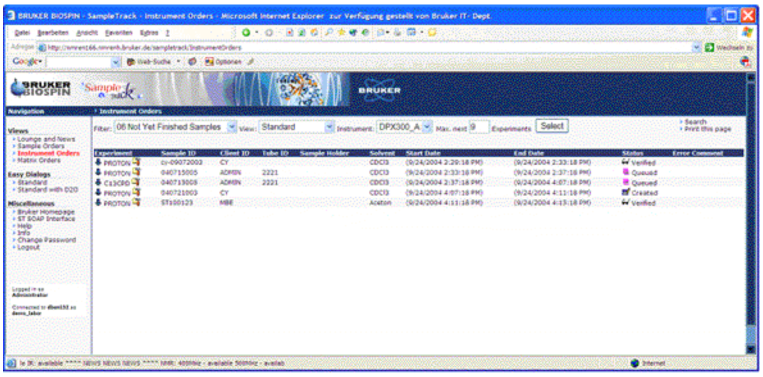
(☐ Please Select.. =) and

Filter: 10 Not Yet Approved Samples View: Standard Samples per page: 12

Instrument Order View 9.2.5

The **Instrument Order View** lets you view experiments that are to be measured in a certain instrument. The filters here are also customizable.

Figure 9.10. Instrument Orders

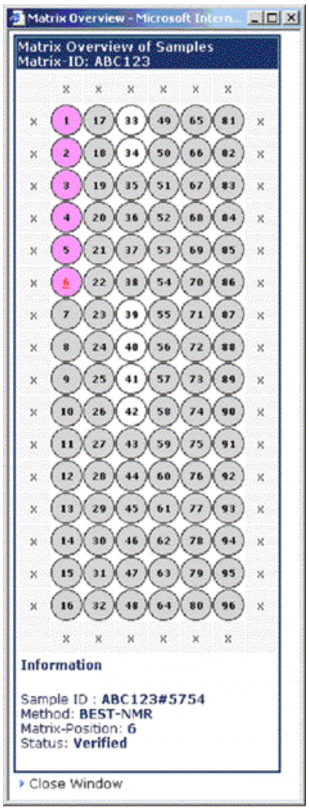


Filter: 06 Not Yet Finished Samples View: Standard Instrument: DPX300_A Max. next 9 Experiments

Experiment	Sample ID	Client ID	Tube ID	Sample Holder	Solvent	Start Date	End Date	Status	Error Comment
PROTON	cy-09072003	CY			CDCl3	(9/24/2004 2:29:18 PM)	(9/24/2004 2:33:18 PM)	Verified	
PROTON	040715005	ADMIN	2221		CDCl3	(9/24/2004 2:33:18 PM)	(9/24/2004 2:37:18 PM)	Queued	
C13CPD	040715005	ADMIN	2221		CDCl3	(9/24/2004 2:37:18 PM)	(9/24/2004 4:07:18 PM)	Queued	
PROTON	040721003	CY			CDCl3	(9/24/2004 4:07:18 PM)	(9/24/2004 4:11:18 PM)	Created	
PROTON	ST100123	MBE			Aceton	(9/24/2004 4:11:18 PM)	(9/24/2004 4:15:18 PM)	Verified	

Matrix Orders 9.2.6

Figure 9.11. Matrix Orders



Matrix Overview of Samples
Matrix-ID: ABC123

1	17	33	49	65	81
2	18	34	50	66	82
3	19	35	51	67	83
4	20	36	52	68	84
5	21	37	53	69	85
6	22	38	54	70	86
7	23	39	55	71	87
8	24	40	56	72	88
9	25	41	57	73	89
10	26	42	58	74	90
11	27	43	59	75	91
12	28	44	60	76	92
13	29	45	61	77	93
14	30	46	62	78	94
15	31	47	63	79	95
16	32	48	64	80	96

Information

Sample ID : ABC123#5754
Method: BEST-NMR
Matrix-Position: 6
Status: Verified

Special matrix orders, e.g. for BEST, can be found with this view.

Enter the matrix ID to find all orders with the leading matrix ID.

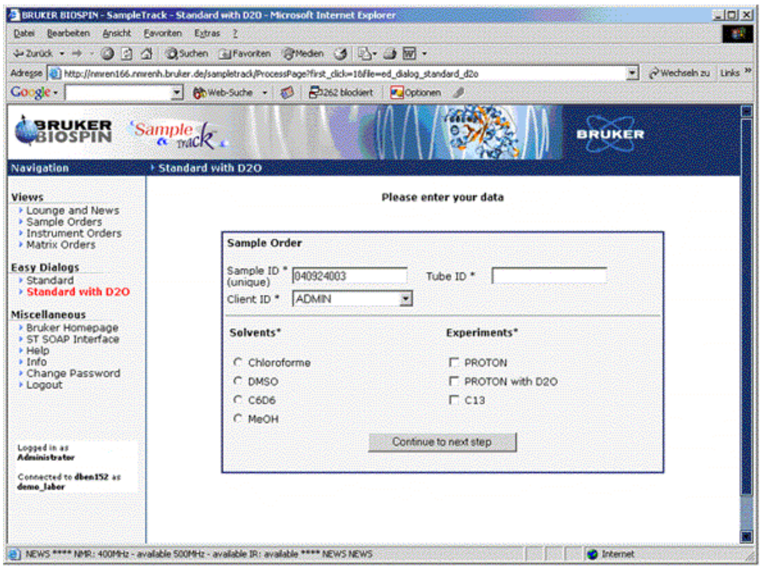
Using the link „Matrix-Overview“ a graphical overview is displayed with a special color for each status of a matrix order.

The worksteps can be diplayed by clicking on the suborder.

Enter Orders Using the EasyWeb Dialog 9.3

On the left navigation board one or several customized order entry forms can be found – **EasyWeb Dialogs**. Those customer interfaces are not connected to the **SampleTrack Client EasyDialog** and must be configured separately.

Figure 9.12. EasyWeb Dialog


BRUKER BIOSPIN - SampleTrack - Standard with D2O - Microsoft Internet Explorer
Datei Bearbeiten Ansicht Favoriten Extras ?
Zurück Suchen Favoriten Medien
Adresse http://nmren166.nmrenh.bruker.de/sampletrack/ProcessPage?first_click=1&file=ed_dialog_standard_d2o
Wechseln zu Links
Google Web-Suche 3262 blockiert Optionen
BRUKER BIOSPIN
Sample Track
BRUKER
Navigation
Standard with D2O
Views
Lounge and News
Sample Orders
Instrument Orders
Matrix Orders
Easy Dialogs
Standard
Standard with D2O
Miscellaneous
Bruker Homepage
ST SOAP Interface
Help
Info
Change Password
Logout
Logged in as Administrator
Connected to dben152 as demo_laber
Continue to next step
NEWS **** NMR: 400MHz - available 500MHz - available IR: available **** NEWS NEWS
Internet

Please enter your data

Sample Order

Sample ID * (unique): 040924003

Tube ID *:

Client ID *: ADMIN

Solvents*

○ Chloroforme
○ DMSO
○ C6D6
○ MeOH

Experiments*

☐ PROTON
☐ PROTON with D2O
☐ C13

The order can be entered on a single page or with a wizard. Only the minimal information is required, usually the method, the solvent and the experiment.

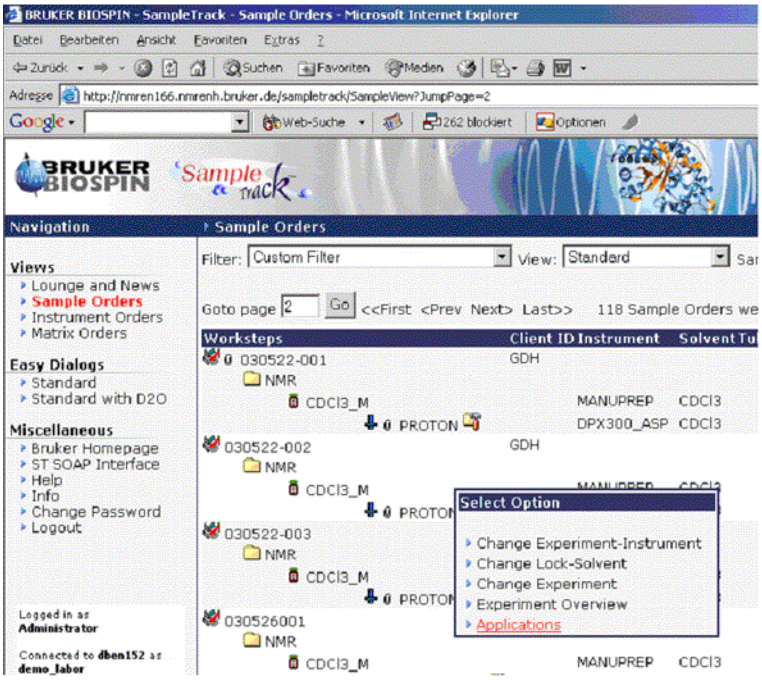
After the entry is made a confirmation window is displayed, where the order can be submitted or modified.

After the submission the new order is displayed.

Applications (only for Windows® Systems) 9.4

The experiment results can be edited with additional applications. In principal it is not possible for security reasons - to start an application from the Web. Therefore the **SampleTrack Application-Wizard** is needed, which starts the selected program with the necessary parameters. Click the experiment Toolbox icon and select “Application” in the following menu.

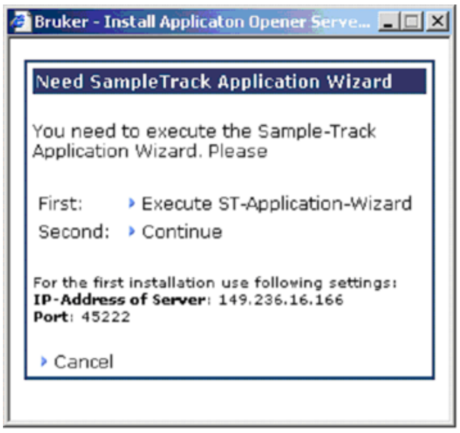
Figure 9.13. Applications


BRUKER BIOSPIN - SampleTrack - Sample Orders - Microsoft Internet Explorer
Datei Bearbeiten Ansicht Favoriten Extras ?
Zurück Suchen Favoriten Medien
Adresse http://nmren166.nmrenh.bruker.de/sampletrack/SampleView?JumpPage=2
Google Web-Suche 262 blockiert Optionen
BRUKER BIOSPIN
SampleTrack
Navigation
Sample Orders
Views
Lounge and News
Sample Orders
Instrument Orders
Matrix Orders
Easy Dialogs
Standard
Standard with D2O
Miscellaneous
Bruker Homepage
ST SOAP Interface
Help
Info
Change Password
Logout
Logged in as Administrator
Connected to dben152 as demo_labor
Filter: Custom Filter
View: Standard
Goto page 2 Go <<First <Prev Next> Last>> 118 Sample Orders we
Worksteps Client ID Instrument Solvent Tu
0 030522-001 GDH
NMR
CDCl3_M MANUPREP CDCl3
0 PROTON DPX300_ASP CDCl3
030522-002 GDH
NMR
CDCl3_M
0 PROTON
030522-003
NMR
CDCl3_M
0 PROTON
030526001
NMR
CDCl3_M MANUPREP CDCl3
Select Option
Change Experiment-Instrument
Change Lock-Solvent
Change Experiment
Experiment Overview
Applications

If the application wizard was not started before, a new window is displayed.

Click „**Execute ST-Application-Wizard**“. When the program appears in the system border, click “Continue”.

Figure 9.14. Application Wizard


Bruker - Install Applicaton Opener Serve...
Need SampleTrack Application Wizard

You need to execute the Sample-Track Application Wizard. Please

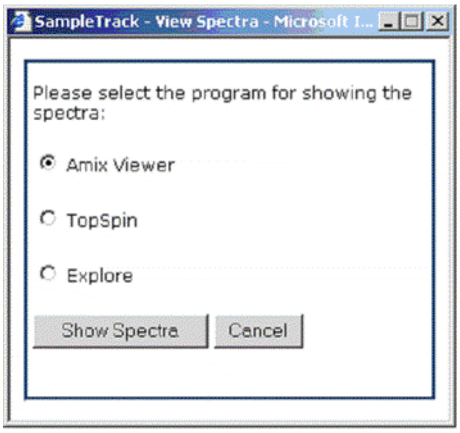
First: Execute ST-Application-Wizard
Second: Continue

For the first installation use following settings:
IP-Address of Server: 149.236.16.166
Port: 45222

To view a spectra, select one of the viewers from the **View Spectra** window.

The program will open and display the spectra in a new window.

Figure 9.15. The View Spectra Window



Please select the program for showing the spectra:

● Amix Viewer

○ TopSpin

○ Explore

Interaction with Automation Robots

10

SampleRail™ 10.1

SampleRail™ is part of a system under the management of SampleTrack™, that automatically prepares an NMR probe, inserts it into an NMR magnet, performs NMR experiments on the probe, and transports it back to the preparation system. The SampleRail™ fulfills the transporting task from the preparation system into the NMR magnet and back while a TECAN® Genesis pipetting robot is used as the preparation system. The SampleRail™ may also be used in a ’manual insertion mode’ to insert/ eject single NMR probes manually into the NMR magnets.

TECAN® - Pooling Module 10.2

The Pooling Module is designed to create special sample orders. These orders contain several worksteps for automation using well plates. The first workstep is to create a preparation of different well plate substances in one tube. The second workstep encompasses the measurement of these substances. After finishing the measurements, the results are interpreted and new sample orders are generated, dependant on the results of the interpretation. Each generation of a new sample order is part of a level. Levels are used to visualize the progress of the automation process. Using the Pooling Module it is very easy to handle large amounts of samples and well plates. The Pooling Module is initially designed for protein screening but can also be used for other applications.

The SampleRail™ is part of a system under the management of the SampleTrack™ Laboratory Information Management System and ICON-NMR™ automation software, that provides automatic preparation and mixing of multiple compounds, and subsequent NMR measurements.

A typical application example is the protein-ligand binding detection by NMR. This system automatically prepares an NMR sample, inserts it into an NMR magnet, performs NMR experiments on the sample, and transports it back to the preparation system.

The SampleRail™ fulfills the transporting tasks from the preparation system into the NMR magnet and back, while a TECAN® GENESIS™ pipetting robot is used as the preparation system. The SampleRail™ may also be used in a **Manual Insertion Mode** to insert and eject single NMR probes manually into the NMR magnets.

TECAN® Requirements *10.2.1*

SampleTrack version 2.35 standard installation.

Stmatrix.bpl and Stpooling.bpl must be installed.

Required SQL tables MATRIX_TABLE and MATRIX_ITEMS must be installed. These are installed automatically beginning with DB release V2.039.

Stmatrix.bpl and Stpooling.bpl must be loaded and configured.

Script library PoolingLib V5.x must be installed.

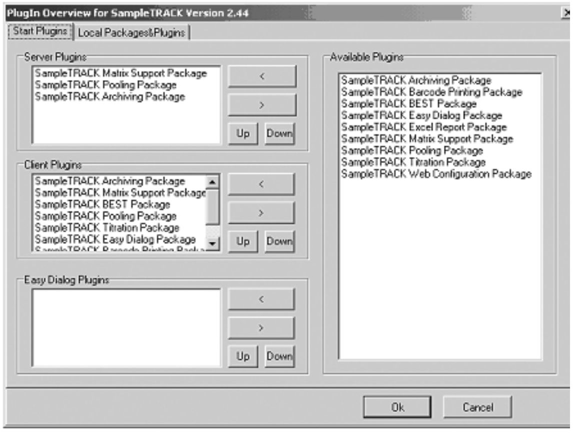
If TECAN® system is present, thescript library TecanLib V5.x must be installed.

Preparation instruments must support the pooling option.

TECAN® Plugin Installation *10.2.2*

Matrix and pooling support are activated using the Configure Plugins window. To open the Configure Plugins window select: Menu->Administration->Configure Plugins. In this window you can add the necessary Stmatrix.bpl and Stpooling.bpl Plugins to SampleTrack Server and Client.

Figure 10.1. Install PlugIns


PlugIn Overview for SampleTRACK Version 2.44
Start Plugins
Local Packages&Plugins
Server Plugins
SampleTRACK Matrix Support Package
SampleTRACK Pooling Package
SampleTRACK Archiving Package
<
>
Up
Down
Client Plugins
SampleTRACK Archiving Package
SampleTRACK Matrix Support Package
SampleTRACK BEST Package
SampleTRACK Pooling Package
SampleTRACK Titration Package
SampleTRACK Easy Dialog Package
<
>
Up
Down
Easy Dialog Plugins
<
>
Up
Down
Available Plugins
SampleTRACK Archiving Package
SampleTRACK Barcode Printing Package
SampleTRACK BEST Package
SampleTRACK Easy Dialog Package
SampleTRACK Excel Report Package
SampleTRACK Matrix Support Package
SampleTRACK Pooling Package
SampleTRACK Titration Package
SampleTRACK Web Configuration Package
Ok
Cancel

Once the PlugIns have been installed, they will need to be configured. This involves two steps:

- Completing the matrix settings
- Completing the pooling settings

TECAN® Matrix Settings *10.2.3*

The first step is to complete the matrix settings. To do this open the Menu->Administration->Options window and select the Matrix Settings tab. Within this tab sheet you can add (or delete) available matrix configurations, by assigning a name and the well plate design, and pressing the Add Matrix Type button. In this tab sheet you should add all the matrix types that will need to be available later for pooling. Matrix type names can be in various forms, based on any established naming conventions.

The following example is based on the classic format used in BEST-NMR:

WH12=hx12

Whereas:

W is for Well plate,

H is a size from A to H, and,

12 is a size from 1 to 12.

WH12 is the name assigned to the configuration

= is a separator

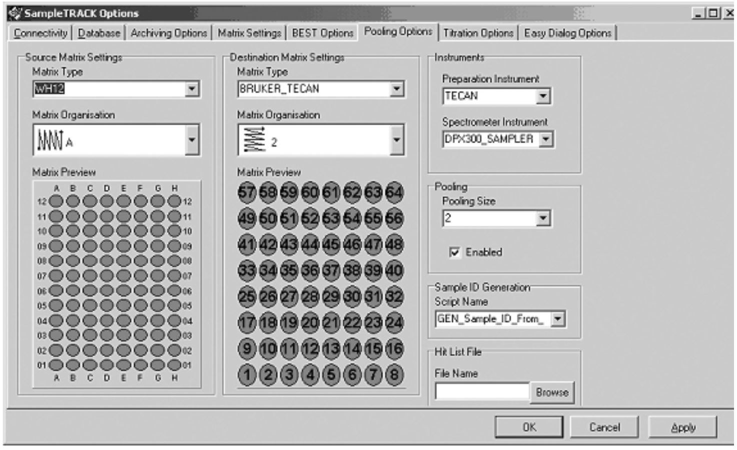
hx12 is the current well plate design

In most laboratories, libraries with well plates are available for protein screening. In order to take advantage of these libraries, an import interface has been designed to import these libraries automatically into the matrix database. To import a library, select an import file and check the 'Enabled' checkbox, which activates the automatic import for the communication server. This information will then be displayed in the information section of the server.

TECAN® Pooling Settings 10.2.4

The second step of the configuration process involves setting the default values for pooling. To do this open the Menu->Administration->Options window and select the Pooling Settings tab sheet. The default settings include the instruments and matrix settings. These values will remain fixed based on the actual instrument configuration. Depending on the kind of matrix type, different matrix organization can be useful. The matrix organization represents from which point to which point each well should be counted to within the well plate. The Pooling Volumes and Pooling Size are flexible values, and can be changed as required.

Figure 10.2. Pooling default values



Source Matrix Settings
Matrix Type: WH12
Matrix Organisation: A

Destination Matrix Settings
Matrix Type: BRUKER_TECAN
Matrix Organisation: 2

Instruments
Preparation Instrument: TECAN
Spectrometer Instrument: DPX300_SAMPLER

Pooling
Pooling Size: 2
☑ Enabled

Sample ID Generation
Script Name: GEN_Sample_ID_From_

Hit List File
File Name:

In most laboratories, libraries with well plates are available for protein screening. In order to take advantage of these libraries, an import interface has been designed to import these libraries automatically into the matrix database. To import a library, select an import file and check the 'Enabled' checkbox, which activates the automatic import for the communication server. This information will then be displayed in the information section of the server.

When you check the 'Enabled' checkbox the automation module in the server is activated. This means that new samples are generated for all samples with hits. This data will be displayed in the beginning of the information section.

TECAN® Instrument Setup 10.2.5

Scripts must be installed and configured for both preparation and experiment instruments. With scripts, the Sample ID is the Matrix ID with a sequence. For file imports and exports the following scripts must be configured:

Instrument	Action	Scripts
Prep Instrument	Export	ASP_EXPORT
		Pooling_Export
Prep Instrument	Import	ASP_IMPORT
		TECAN_WORKAROUND (if prep instrument is
		TECAN system)
Exp Instrument	Export	AVANCE_Export
		Pooling_Export
Exp Instrument	Import	AVANCE_Import
LIMS Instrument	Import	GEN_SAMPLE_ID
		LIMS_Import_SO_Pooling_Defaults
		LIMS_Import_SO_Pooling

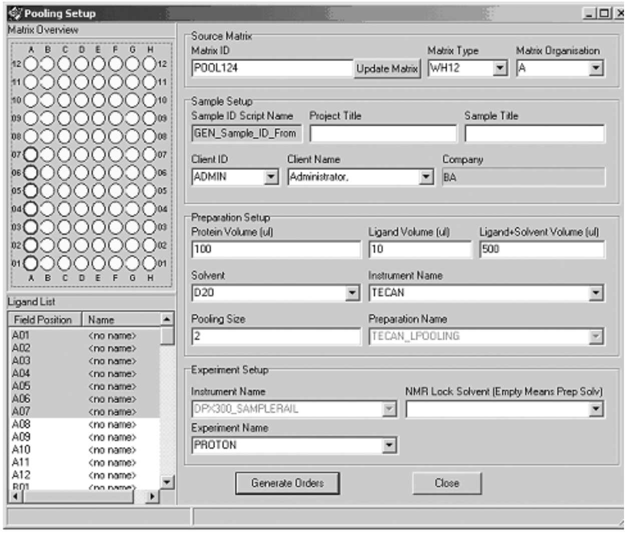
The script GEN_SAMPLE_ID creates an unique identifier for samples, with the MATRIX_ID as the prefix and MATRIX_SEQ as the sequence.

Protein Screening / Module Pooling 10.3

TECAN® Generating Samples 10.3.1

The dialog for sample setup is started when you press the ’New’ button in the Pooling Orders Window. Here you can enter the well plate for pooling, and select the wells that are to be used by clicking on them with your mouse. After entering the Project Title, Sample Title and Experiment Name, press the Generate Order button to generate the sample orders. Worksteps with tubes will be created based on the pooling size. This level is also referred to as level 0. If Matrix ID specific information is imported from the communication server, the Ligand's are displayed in the Ligand list in the table BSTS_REGISTRY.

Figure 10.3. Protein Screening / Module 'Pooling'



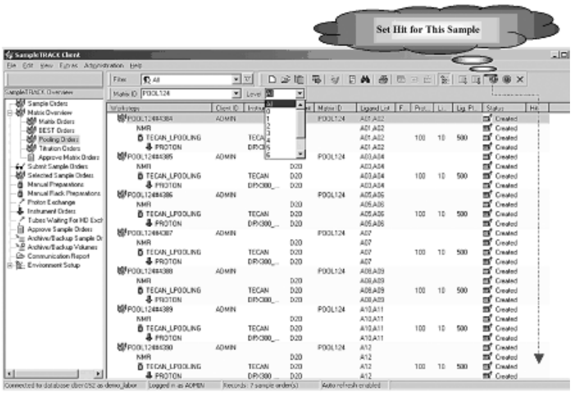
Matrix ID: POOL124
Matrix Type: WH12
Matrix Organisation: A
Sample ID Script Name: GEN_Sample_ID_From
Project Title:
Sample Title:
Client ID: ADMIN
Client Name: Administrator,
Company: BA
Protein Volume (ul): 100
Ligand Volume (ul): 10
Ligand+Solvent Volume (ul): 500
Solvent: D20
Instrument Name: TECAN
Pooling Size: 2
Preparation Name: TECAN_LPOOLING
Instrument Name: DPX300_SAMPLERAIL
NMR Lock Solvent (Empty Means Prep Solv):
Experiment Name: PROTON

Field Position	Name
A01	<no name>
A02	<no name>
A03	<no name>
A04	<no name>
A05	<no name>
A06	<no name>
A07	<no name>
A08	<no name>
A09	<no name>
A10	<no name>
A11	<no name>
A12	<no name>
B01	<no name>

TECAN® Starting the Automation Process **10.3.2**

Before a new automation process can be started, all currently running automation processes must be stopped. This means the Tecan® Genesis System must be reset to its initialization state, and ICON-NMR™ must be reset. Following this step the Pooling Setup window will be closed and the updated sample list for this Matrix ID should be visible.

Figure 10.4. Setting hits



Press **Select All** or **CTRL A** and submit all the samples. The initial level is 0 with 4 substances. At this point all of the samples are ready for automation. Once all the samples have been submitted, the worksteps will be run automatically.

After the experiments are finished, the data can be viewed with the available spectra viewer and a decision can be made if the samples are hits or not. If the samples are hits, then the corresponding checkboxes can be selected for these samples. The next step (level), with 2 substances per sample, can be executed by pressing the Execute button. Protein Imaging is finished when all the samples with hits have been measured with only one substance.

Environment Setup

11

SampleTrack™ Environment Setup 11.1

The SampleTrack™ Environment Setup module of the SampleTrack™ Overview allows existing information from the user, instruments etc., to be defined or modified. To avoid unwanted deletions or modifications to the setup parameters, access to this section should be limited to the System Administrator.

Inserting a New User in the Companies Setup Module 11.2

The Companies setup module allows you to insert new users in the SampleTrack™ system. This process can basically be broken down into three steps:

Step One: Inserting a New Company***"Inserting a New Company" on page 86***

Step Two: Entering a New Department***"Entering a New Department" on page 87***

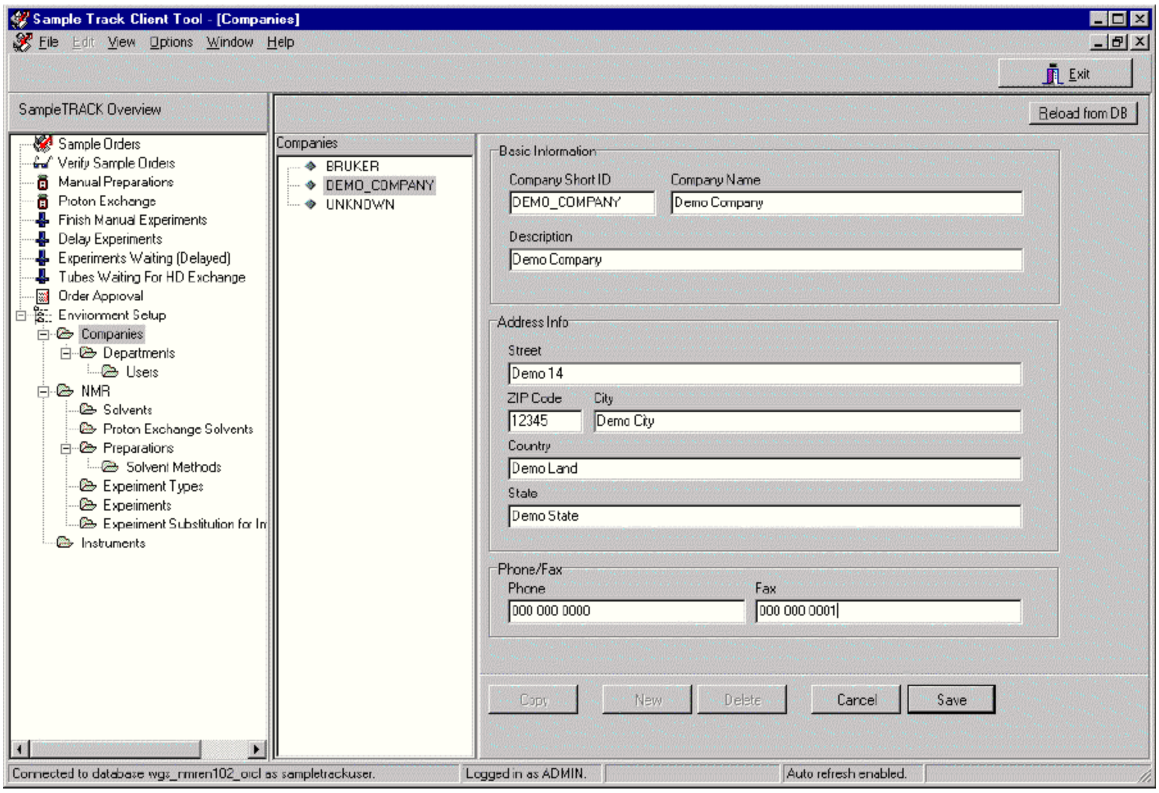
Step Three: Entering a New User***"Entering a New User" on page 88***

Inserting a New Company 11.3

As some laboratories have users from various companies, the first step is to determine if the new user's company exists on the **Companies** list. When not, a new company entry can be added to the list:

- Highlight **Companies** in the Environment Setup.
- Press the **New** button.
- Fill out the data blocks.
- Press **Save** to enter the new information in the list.

Figure 11.1. Environment Setup



Company Short ID: DEMO_COMPANY
Company Name: Demo Company
Description: Demo Company
Street: Demo 14
ZIP Code: 12345
City: Demo City
Country: Demo Land
State: Demo State
Phone: 000 000 0000
Fax: 000 000 0001

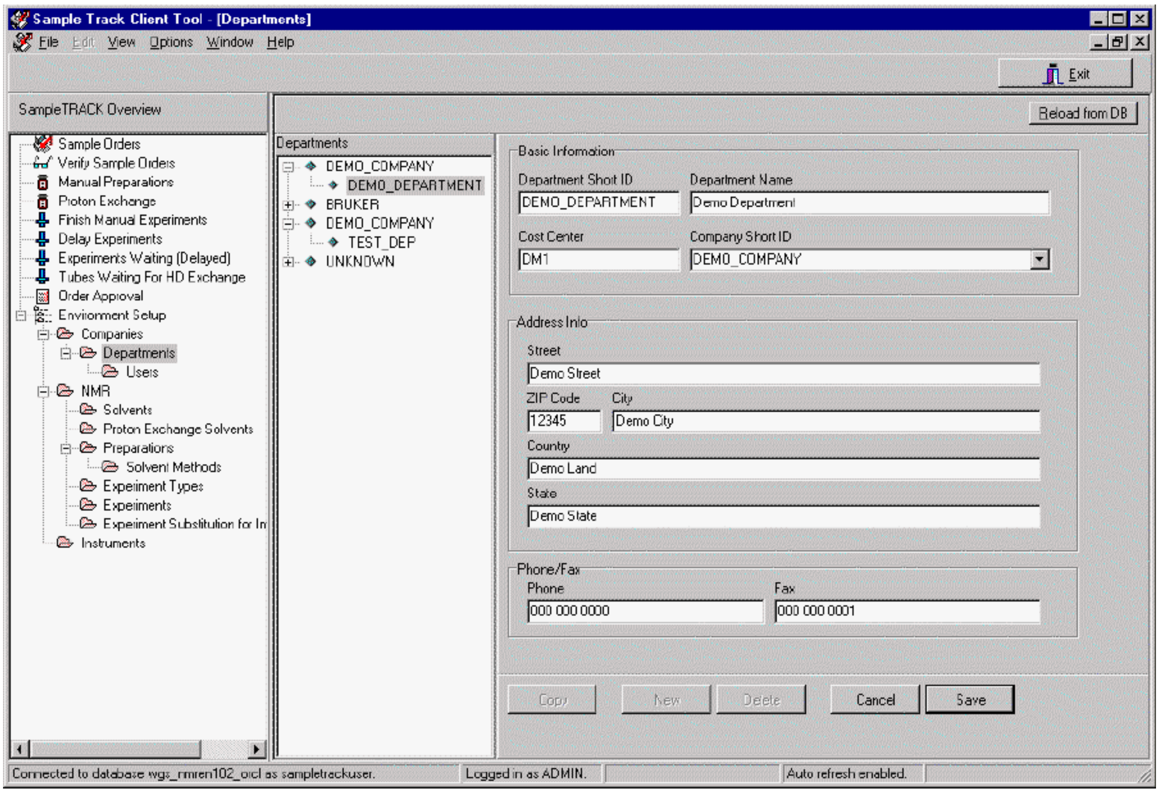
Connected to database wgs_rmren102_orcl as sampletrackuser.
Logged in as ADMIN.
Auto refresh enabled.

Entering a New Department *11.4*

The next step in inserting a new user is to determine if the new user's department exists on the **Departments** list. As before, if the Department doesn't exist a new department can be added to the list:

- High-light **Departments** in the Environment Setup.
- Press the **New** button.
- Fill out the data blocks.
- Press **Save** to enter the new information in the list.

Figure 11.2. New Department



Department Short ID: DEMO_DEPARTMENT
Department Name: Demo Department
Cost Center: DM1
Company Short ID: DEMO_COMPANY
Street: Demo Street
ZIP Code: 12345
City: Demo City
Country: Demo Land
State: Demo State
Phone: 000 000 0000
Fax: 000 000 0001

Connected to database wgs_nmren102_orcl as sampletrackuser. | Logged in as ADMIN. | Auto refresh enabled.

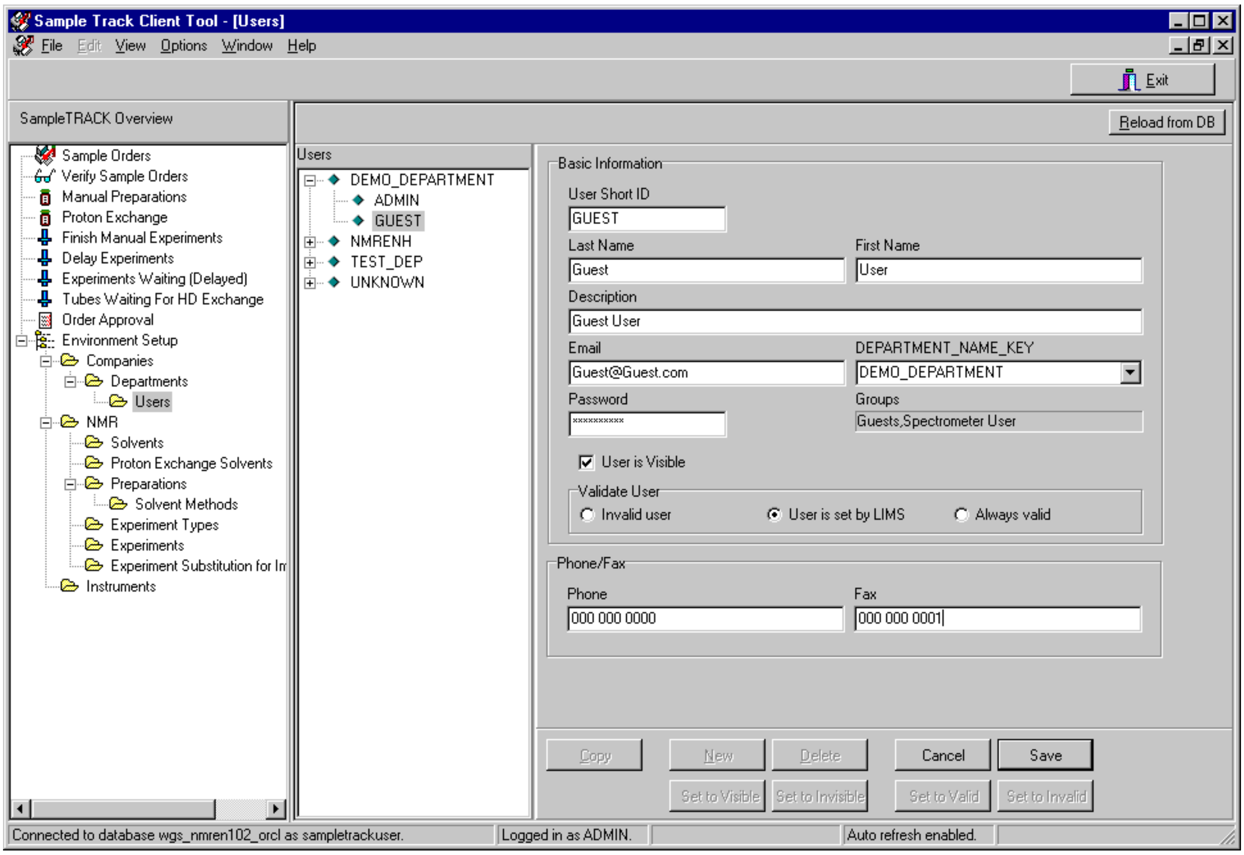
Entering a New User *11.5*

Once you have selected the new users company and department, enter the new user:

- High-light **Users** in the Environment Setup.
- Press the **New** button.
- Fill out the data blocks.
- Press **Save** to enter the new information in the list.

Note: In each of the cases mentioned above you can speed the entry process by finding a company, department or user with similar data and using Copy to create a new entry, whereas you must only edit the data. To insert a new entry DO NOT simply select a present user and edit the entry, as this will only edit that entry, not create a new one. Always use **New** or **Copy** to create an entry!

Figure 11.3. New User



Basic Information

User Short ID: GUEST

Last Name: Guest

First Name: User

Description: Guest User

Email: Guest@Guest.com

DEPARTMENT_NAME_KEY: DEMO_DEPARTMENT

Password: **********

Groups: Guests,Spectrometer User

☑ User is Visible

Validate User: ○ Invalid user ● User is set by LIMS ○ Always valid

Phone/Fax

Phone: 000 000 0000

Fax: 000 000 0001

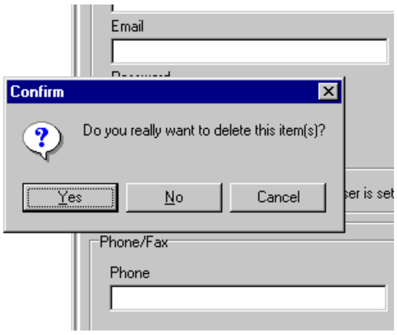
Connected to database wgs_nmren102_orcl as sampletrackuser. | Logged in as ADMIN. | Auto refresh enabled.

Deleting a User, Department, or Company 11.6

A company can only be deleted when all of the departments have been deleted. In turn, a department can only be deleted when all users within the department have been deleted. In any case discretion should be used in who has access to this section. Generally, only the system administrative should be assigned this privilege.

To delete an entry, highlight the entry with your mouse and press **Delete**. You will prompted for a confirmation, press Yes if you are sure you want to delete the entry.

Figure 11.4. Message: Delete?



Do you really want to delete this item(s)?

Inserting a New Instrument 11.7

Important: The insertion of new instruments should normally be carried out only by trained Bruker personnel. An improper insertion or modification of an instrument can result in a communication failure.

A new instrument is added to the **Instruments** list by pressing the New button and completing the necessary entries for **Common Settings**, **Communication Paths & Files** and **Spectrometer Settings**. The new instrument is saved to the list by pressing the **New** button.

Again a word of warning, incorrect parameters will result in improper or no communication!

Inserting a New Method Type 11.8

The **Method Type** serves the purpose of providing a short description of the various type of preparation methods that are available. As new methods are supported, they can also be described here.

Inserting a New Solvent 11.9

In most cases solvents and experiments are maintained within the spectrometer software, e.g. ICON-NMR™ or external LIMS. **They are imported automatically into the SampleTrack™ system**.

The **Solvents** block under NMR provides information on the instruments and their solvents that are currently defined. To insert a new solvent:

- Highlight **Solvents.**
- Select the appropriate instrument (e.g. DPX300) from the **Instruments & Solvents** block.
- Press **New** and fill in the required data.
- Press **Save** to add the new solvent entry to the instrument that you have selected.

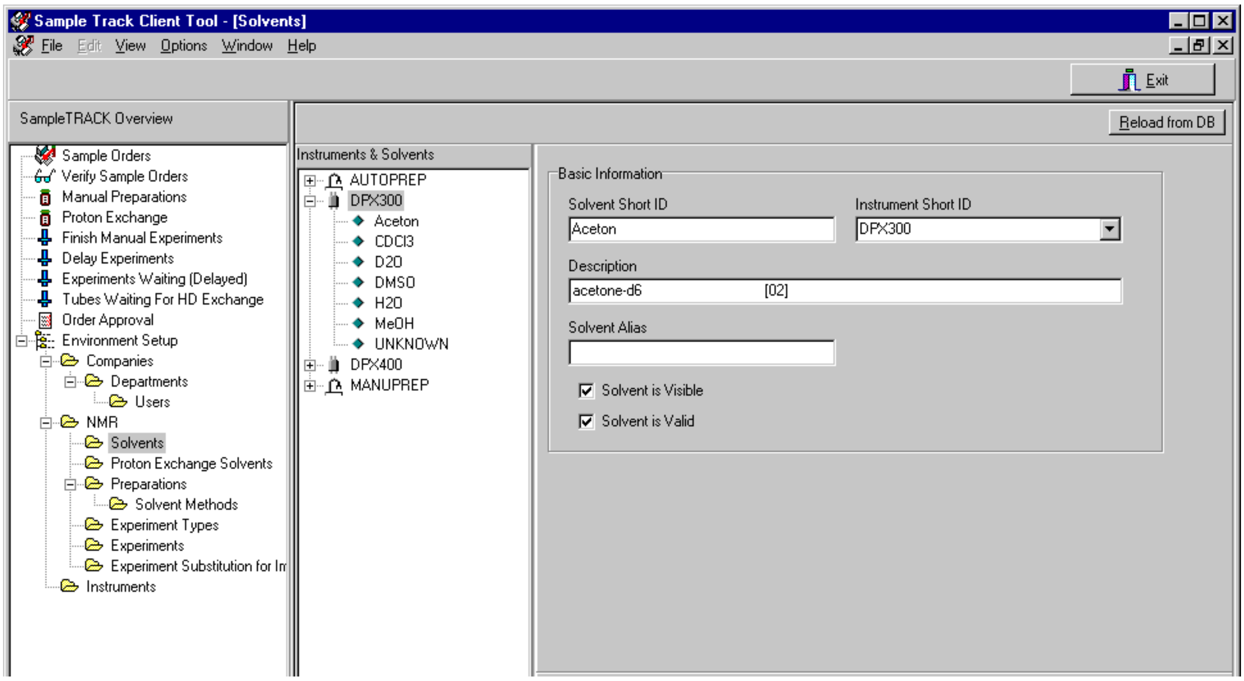
Solvent is Visible

When entering a new solvent you will notice two checkboxes, **Solvent is Visible** and **Solvent is Valid**. At times it may be desirable to make a solvent temporarily unavailable to a user. Deselecting the **Solvent is Visible** box will hide this option from the user, the user will not be able to select the solvent. Checking the box will return the solvent to the list of options.

Solvent is Valid

When a solvent will no longer be used for experiments you can not simply delete it, as previous experiments may still have a reference link to the solvent. Instead the **Solvent is Valid** box should be deselected, which will delete the solvent from the list of solvents that are available. The solvent can be reinstated at a later time by rechecking the box.

Figure 11.5. New Solvent



Basic Information

Solvent Short ID: Aceton

Instrument Short ID: DPX300

Description: acetone-d6 [02]

Solvent Alias:

☑ Solvent is Visible

☑ Solvent is Valid

Inserting a Proton Exchange Solvent *11.10*

The solvents listed in this module represent all of the proton exchange solvents that have been defined for manual preparations (only).

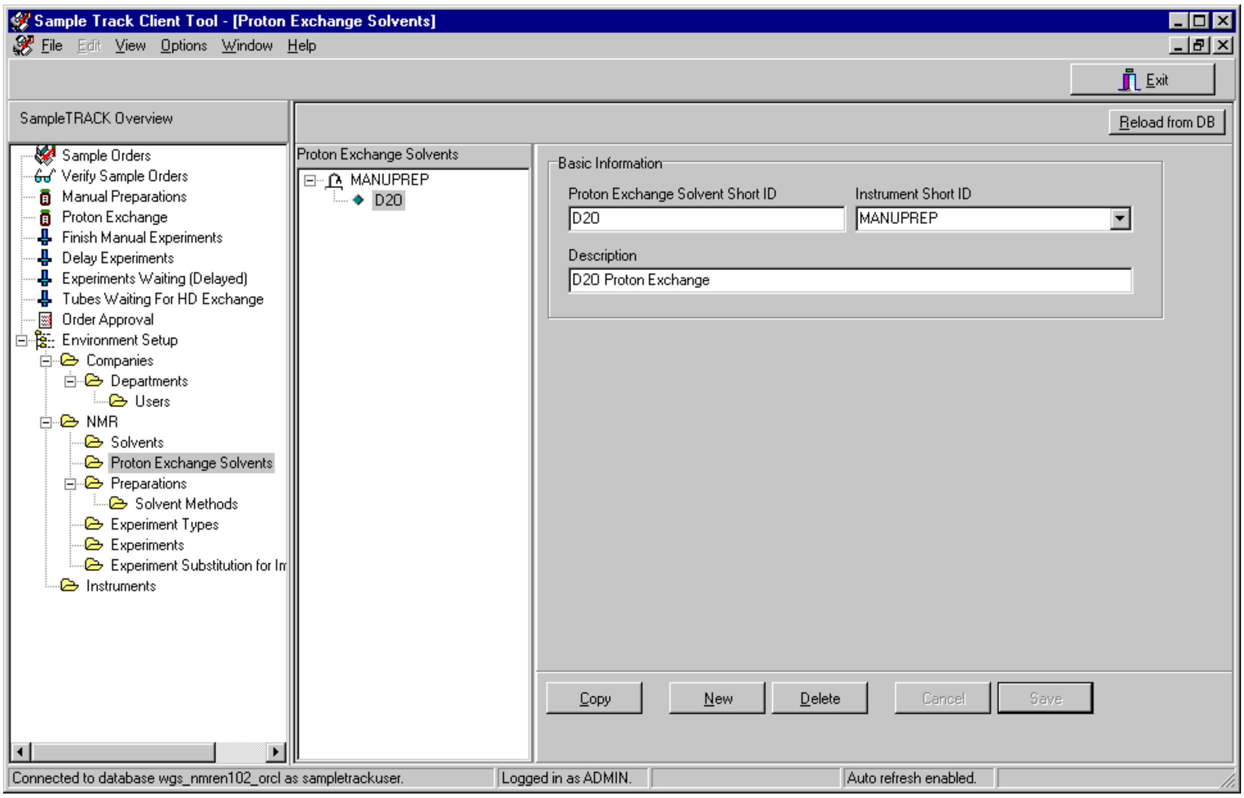
To insert a new solvent entry:

Highlight **Proton Exchange Solvents.**

Press **New** and enter the requested data.

Press **Save** to add the new solvent to the list.

Figure 11.6. New Proton Exchange Solvent



Proton Exchange Solvent Short ID: D2O

Instrument Short ID: MANUPREP

Description: D2O Proton Exchange

Connected to database wgs_nmren102_orcl as sampletrackuser.

Logged in as ADMIN.

Auto refresh enabled.

Inserting a New Preparation Method 11.11

This module allows you to pre-define new preparation methods. To configure a new preparation:

Highlight **Preparations.**

Select the relevant instrument.

Press the **New** button.

Fill out the requested data.

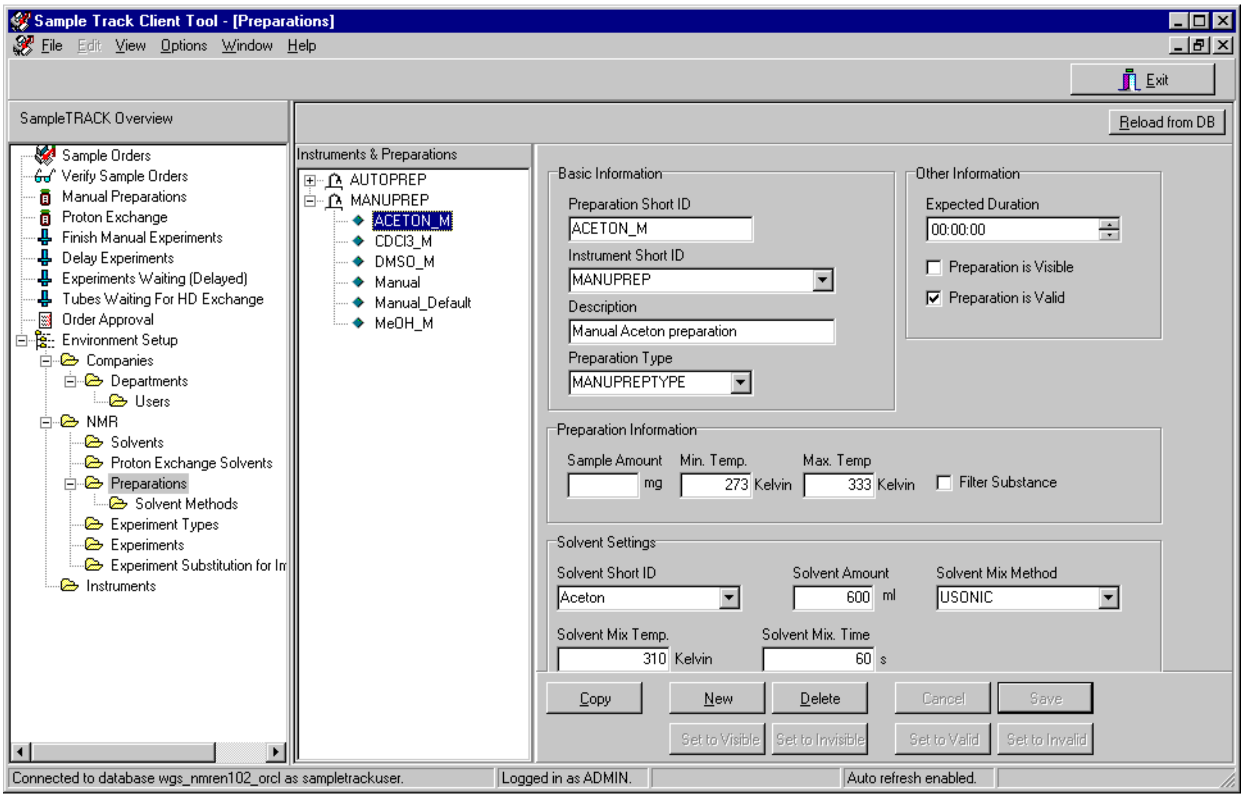
Press **Save** to add the preparation method to the list.

Preparation is Visible, Preparation is Valid

As was true with the insertion of a solvent module, the **Preparation**, **Solvent Methods**, and **Experiments** modules also have **Visible and Valid** checkboxes.

The same rules apply for those checkboxes as those for the solvent module.

Figure 11.7. New Preparation Method



Basic Information
Preparation Short ID: ACETON_M
Instrument Short ID: MANUPREP
Description: Manual Aceton preparation
Preparation Type: MANUPREPTYPE

Other Information
Expected Duration: 00:00:00
☐ Preparation is Visible
☑ Preparation is Valid

Preparation Information
Sample Amount: mg
Min. Temp.: 273 Kelvin
Max. Temp: 333 Kelvin
☐ Filter Substance

Solvent Settings
Solvent Short ID: Aceton
Solvent Amount: 600 ml
Solvent Mix Method: USONIC
Solvent Mix Temp.: 310 Kelvin
Solvent Mix. Time: 60 s

Connected to database wgs_nmren102_orcl as sampletrackuser. | Logged in as ADMIN. | Auto refresh enabled.

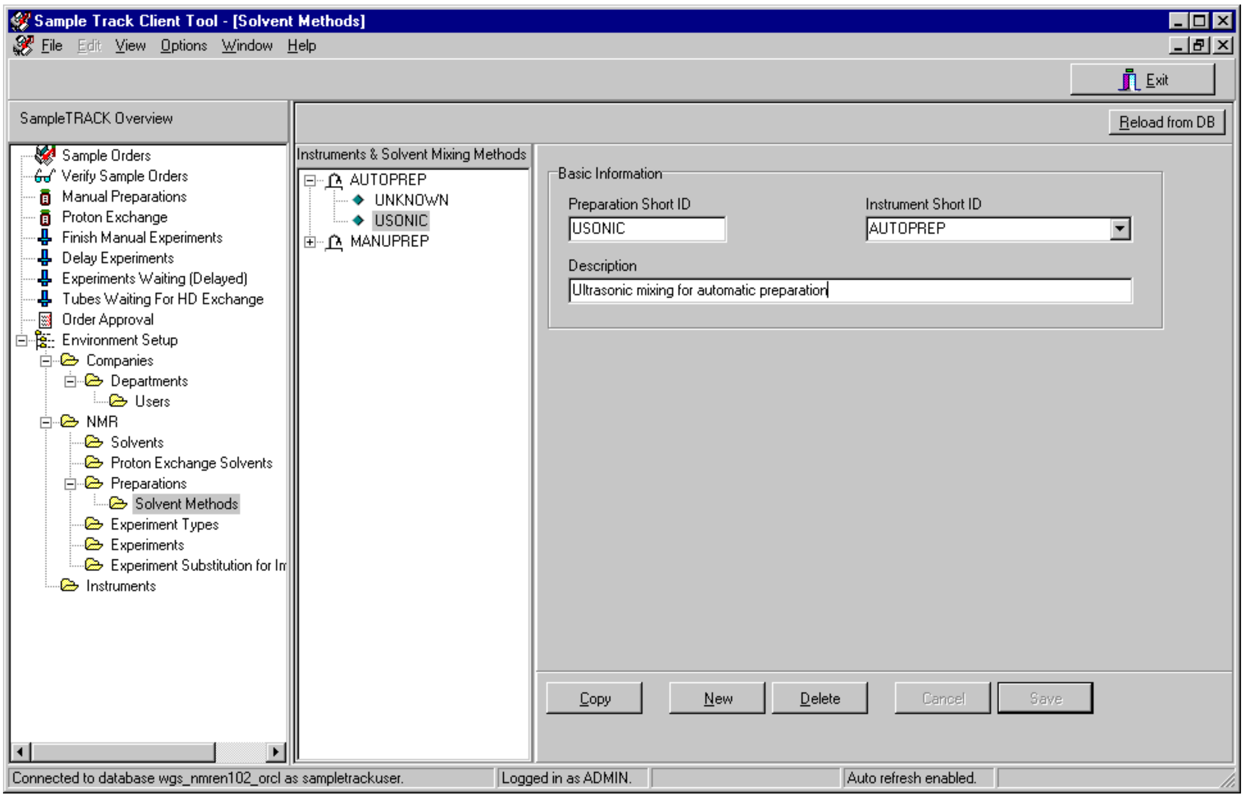
Inserting a Solvent Mixing Method *11.12*

The **Solvent Methods** section under **Preparations** allows you to configure solvent mixing methods for a preparation. Again this is accomplished by highlighting **Solvent Methods**, selecting the appropriate instrument, pressing New and filling out the request data blocks. The entry is added to the list by pressing the Save button.

To do this:

- Highlight **Solvent Methods.**
- Select the appropriate instrument.
- Press **New** and fill in the required data.
- Press **Save** to add the new solvent mixing method.

Figure 11.8. New Solvent Mixing Method



Preparation Short ID: USONIC

Instrument Short ID: AUTOPREP

Description: Ultrasonic mixing for automatic preparation

Connected to database wgs_nmren102_orcl as sampletrackuser.

Logged in as ADMIN.

Auto refresh enabled.

Inserting New Experiments 11.13

In most cases solvents and experiments are maintained within the spectrometer software, e.g. ICON-NMR™ or external LIMS. They are imported automatically into the SampleTrack™ system.

When the spectrometer AU program is started, data on the experiments that are available are exported to SampleTrack™. The **Experiments** module allows you to define new experiments for spectrometers (only). This step requires that the new experiment is recognized by the spectrometer, i.e. it must be an experiment predefined for that spectrometer.

To insert a **new experiment**:

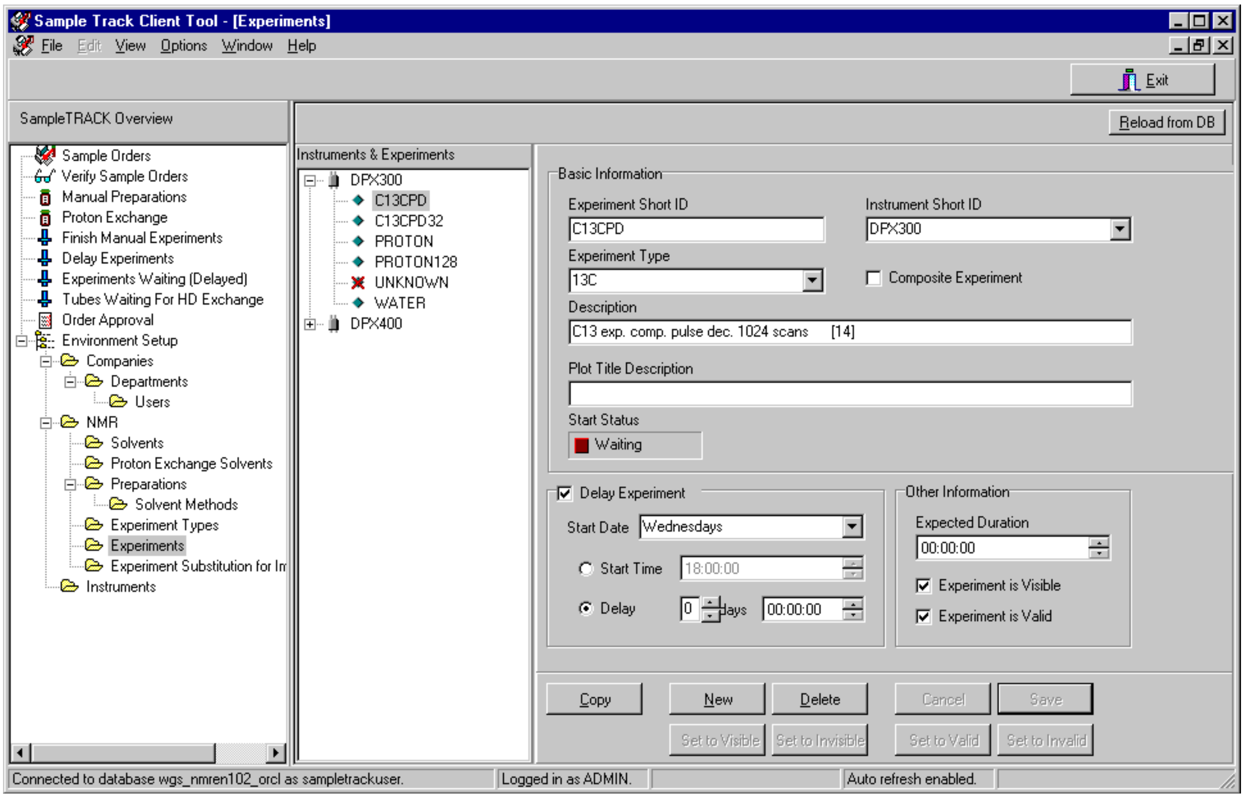
Highlight **Experiments**.

Select the required instrument (a spectrometer in any case).

Press **New** and enter the appropriate parameters.

Press **Save** to add the entry to the list of experiments.

Figure 11.9. New Experiment



Experiment Short ID: C13CPD

Instrument Short ID: DPX300

Experiment Type: 13C

☐ Composite Experiment

Description: C13 exp. comp. pulse dec. 1024 scans [14]

Plot Title Description:

Start Status: Waiting

☑ Delay Experiment

Start Date: Wednesdays

○ Start Time 18:00:00

● Delay 0 days 00:00:00

Expected Duration: 00:00:00

☑ Experiment is Visible

☑ Experiment is Valid

Connected to database wgs_nmren102_orcl as sampletrackuser. | Logged in as ADMIN. | Auto refresh enabled.

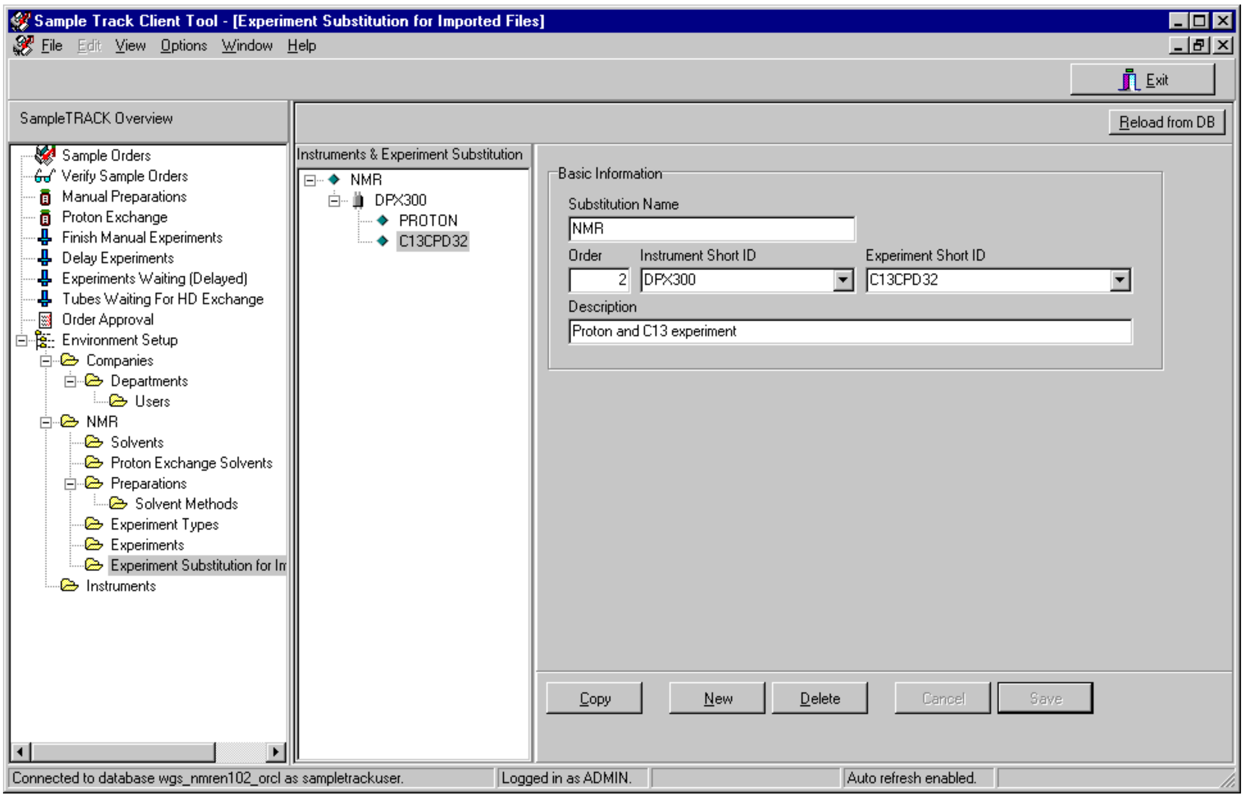
Experiment Substitution for Imported Files *11.14*

In some cases it may be necessary or desirable to use a substitute name for an experiment. For example, with a C13 experiment, the problem exists that the LIMS lists the experiment as C13, while the spectrometer recognizes the experiment as C13CPD. This naming problem can be eliminated by assigning an alias through this module. This module creates, in effect, an Experiment Translation Table.

Furthermore, this module allows you to assemble a group of experiments together under one experiment name. This allows you to perform a variety of experiments under one experiment title. For example, the figure below illustrates an experiment "Test". Grouped under this experiment are two experiments, a **PROTON** and a **C13CPD**. When you create a new grouping (highlight **Experiment Substitution for Imported Files**, select an Instrument, press New) the order in which the experiments will be carried out is determined as you add new experiments (in the **Order** box). Upon saving this experiment group you must only select the experiment "Test" to carry out both the PROTON and C13CPD experiments.

Assembling a Group of Experiments Under One Title

Figure 11.10.Experiment Substitution Table



Sample Track Client Tool - [Experiment Substitution for Imported Files]

Substitution Name: NMR

Order: 2

Instrument Short ID: DPX300

Experiment Short ID: C13CPD32

Description: Proton and C13 experiment

Connected to database wgs_nmren102_orcl as sampletrackuser.

Logged in as ADMIN.

Auto refresh enabled.

The Object Manager

12

Introduction to the Object Manager

12.1

When SampleTrack™ is first installed, a set of default user groups is installed in the Object Manager. The administrator must then adjust these group client profiles (or add new groups) to meet the needs of their individual laboratory. The Object Manager allows the administrator to quickly and easily administer the privileges and work areas of groups of users.

Normally each user belongs to at least the most basic group, the **All User Group**. This group is assigned a basic set of user privileges which allow them to perform the most common tasks in SampleTrack™. Additional privileges can be granted to a user by assigning them to another existing group that has these privileges, by changing the rights of the entire group that they are currently in, or by creating a new group that contains the privileges that they require.

When modifying an existing group, or adding a new group, there are four main configuration areas that must be addressed. These include the Client Profile, Table Defaults, Easydialog and Filter Modules.

The Client Profile is basically a set of rights and privileges that are assigned to a group of users in regards to their use of SampleTrack™ and the laboratory automation. The rights that are assigned a group are based on the needs of the group of users and the standard policies of the individual laboratory.

The Table Default settings are used to create default starting values for various field entries within the tables in SampleTrack™.

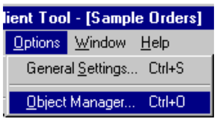
The EasyDialog configuration is the pre-defined EasyDialog configuration that the group of users will be using (see the chapter on configuring EasyDialog***"Opening the EasyDialog Configuration Window" on page 123***).

The Filter Modules are a selection of pre-defined or user-defined filters that are assigned to the group.

Opening the Object Manager 12.2

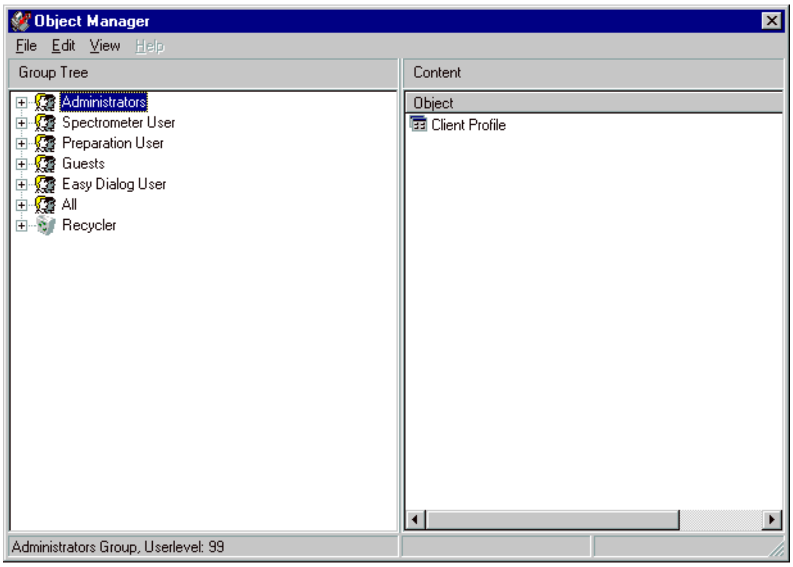
To open the object manager you must be logged-in to the SampleTrack™ Client Tool as administrator. Select Options - Object Manager from the main pull-down menu as shown in the figure below:

Figure 12.1. Menu Object Manager



The Object Manager window shown below will open. If you are opening the Object Manager for the first time, e.g. right after the installation of SampleTrack™, the window will contain default entries in the Group Tree and Content frames. These entries will need to be adjusted based on your client needs.

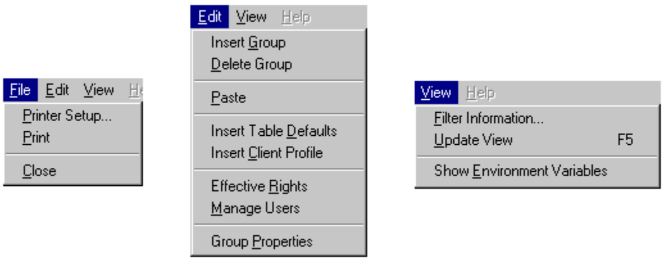
Figure 12.2. Object Manager Main Window



The Object Manager Main Menu 12.3

The Object Manager main menu contains three main sections: File, Edit, and View; and a Help section. The File menu section contains a Microsoft Windows® standard Printer Setup, a Print selection that allows you to print the present screen, and a Close selection which closes the Object Manager.

Figure 12.3. Maintaining Groups



The main menu option Edit contains a group of selections that relate directly to the administration facilities of the Object Manager. The following list is a quick description of each selection.

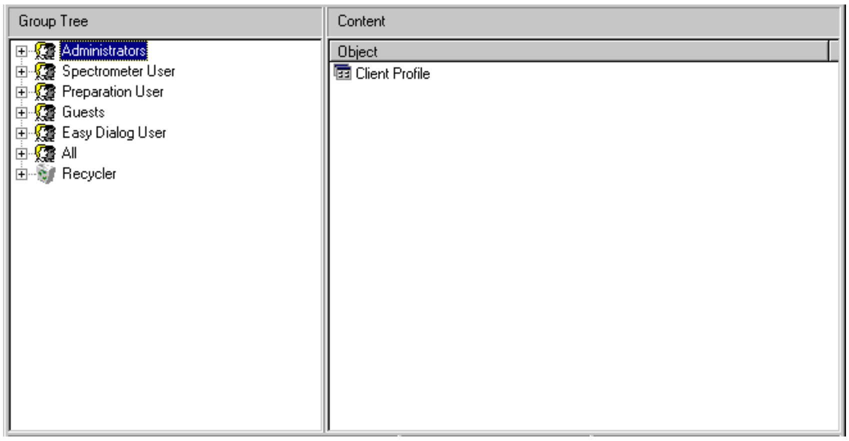
Insert Group:	Used to create a new user group.
Delete Group:	Used to delete a work group.
Paste:	This is a Windows® standard paste routine that can be used to paste data from one group or individual to another, or from an external source (e.g. Clipboard).
Insert Table Defaults:	Used to create default starting values for various field entries within the tables in SampleTrack™.
Insert Client Profile:	Used for establishing a new client profile.
Effective Rights:	Used to provide a quick overview of the rights that are currently assigned to an individual or group.
Manage Users:	Used to add or delete users from a group.
Group Properties:	Used to assign properties to a group (e.g. group name, description and user level).
The main menu option View	Contains selections that relate to the overview of the Object Manager window.
Filter Information:	Used to select which information will be displayed in the Object Manager window.
Update View:	Refreshes the information in the Object Manager window.
Show Environment:	Displays the current attributes that are assigned to the groups
Variables:	The present environment.

The Group Tree and Content Sub-windows 12.4

The Group Tree and Content sub-windows function similarly to the File Manager of Microsoft Windows®. The groups are displayed in the Group Tree, and the details (or contents) of the groups are displayed in the Content window.

When SampleTrack™ is first installed a number of default groups are created. As the following figure illustrates, these groups contain various sub-categories including Client Profiles, Module Sample Orders (filter information), Table Defaults and EasyDialog configurations.

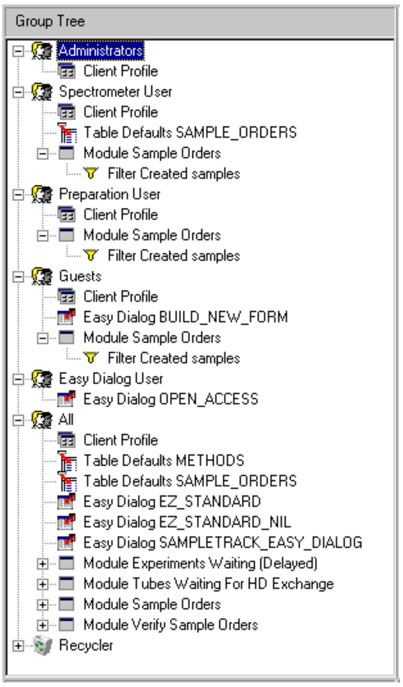
Figure 12.4. Content Sub-Window



- Administrators
- Spectrometer User
- Preparation User
- Guests
- Easy Dialog User
- All
- Recycler

Client Profile

Figure 12.5. Default Groups

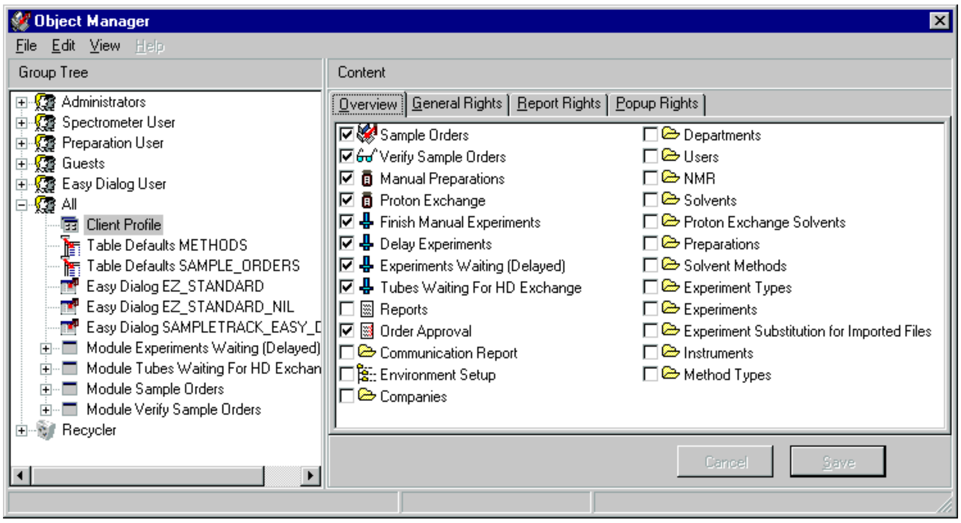


- Administrators
  - Client Profile
- Spectrometer User
  - Client Profile
  - Table Defaults SAMPLE_ORDERS
  - Module Sample Orders
    - Filter Created samples
- Preparation User
  - Client Profile
  - Module Sample Orders
    - Filter Created samples
- Guests
  - Client Profile
  - Easy Dialog BUILD_NEW_FORM
  - Module Sample Orders
    - Filter Created samples
- Easy Dialog User
  - Easy Dialog OPEN_ACCESS
- All
  - Client Profile
  - Table Defaults METHODS
  - Table Defaults SAMPLE_ORDERS
  - Easy Dialog EZ_STANDARD
  - Easy Dialog EZ_STANDARD_NIL
  - Easy Dialog SAMPLETRACK_EASY_DIALOG
  - Module Experiments Waiting (Delayed)
  - Module Tubes Waiting For HD Exchange
  - Module Sample Orders
  - Module Verify Sample Orders
- Recycler

Viewing Group Details in the Content Window 12.5

When you select one of the groups or group sub-category in the Group Tree, the contents will appear in the Content window. For example, if I select the Client Profile for group **All** the following contents will be displayed in the Content window:

Figure 12.6. Group Tree



☑ Sample Orders
☑ Verify Sample Orders
☑ Manual Preparations
☑ Proton Exchange
☑ Finish Manual Experiments
☑ Delay Experiments
☑ Experiments Waiting (Delayed)
☑ Tubes Waiting For HD Exchange
☐ Reports
☑ Order Approval
☐ Communication Report
☐ Environment Setup
☐ Companies
☐ Departments
☐ Users
☐ NMR
☐ Solvents
☐ Proton Exchange Solvents
☐ Preparations
☐ Solvent Methods
☐ Experiment Types
☐ Experiments
☐ Experiment Substitution for Imported Files
☐ Instruments
☐ Method Types

Client Profile Example 12.6

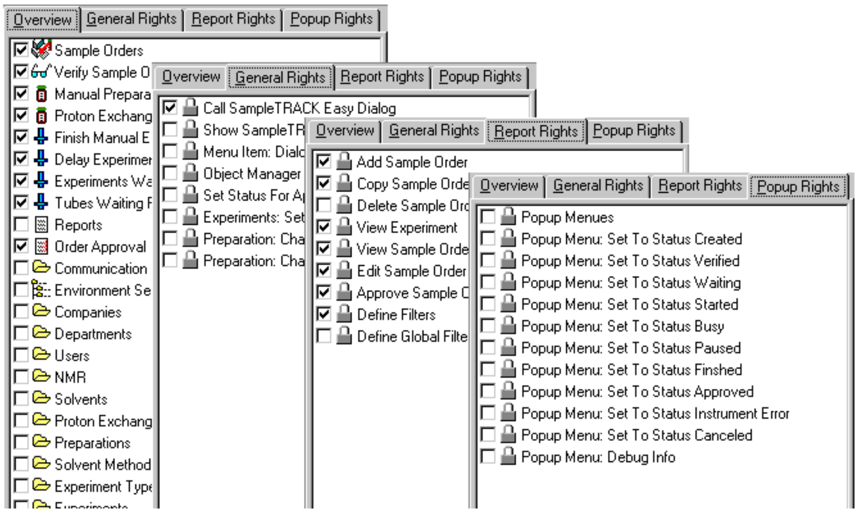
When viewing the Client Profile, four separate window views containing various rights are available in the Content window, as shown in the figure below:

By selecting/deselecting the various rights, the administrator can quickly establish a SampleTrack™ Client Profile. You will notice that each group has a client profile, where the administrator can assign specific rights for that specific group. The concept of user classification and client profiles will be discussed in further detail in the next section.

When you click on another sub-category of the Group Tree a different set of data will be displayed in the Content window. Each sub-category has its own unique details, thus the Content window will change as you move from one tree node to another.

This should be familiar for anyone who has worked with the Microsoft® Windows® File Manager.

Figure 12.7. Sub-categories



User Classification and Client Profiles 12.7

Each user group has its own Client Profile, which consists of a selection of access privileges to various elements of SampleTrack™. These client access privileges are granted to all the users within a group. In most cases, a basic access configuration is established that applies to every user, then additional privileges are assigned to specific workgroups as needed. This allows the administrator to control the flow of samples to the various laboratory automation (e.g. Spectrometers) by assigning users to various groups based on their access requirements.

Each client profile can be assigned a user level. The lowest user level **00**, is the **All** profile. The highest user level, **99** is generally reserved for the system administrator. A new group client profile is automatically assigned the next available user level number when the profile is created. This level can be adjusted later on by the administrator in the Group Properties window.

The user level privileges are inheritable, whereby a user who is part of a higher level user group (parent) inherits the privileges from any lower level group (child) that they are also a member of. For example, if I have a user "Joe Tester" that is in a group called "Spectrometer User" which has user level 04, and also is a member of the group "Preparation User" which has a user level 03, the user "Joe Tester" would have all of the privileges of the Spectrometer User group, the Preparation User group and the basic group: **All**. This will become more apparent as we discuss the details of the object manager.

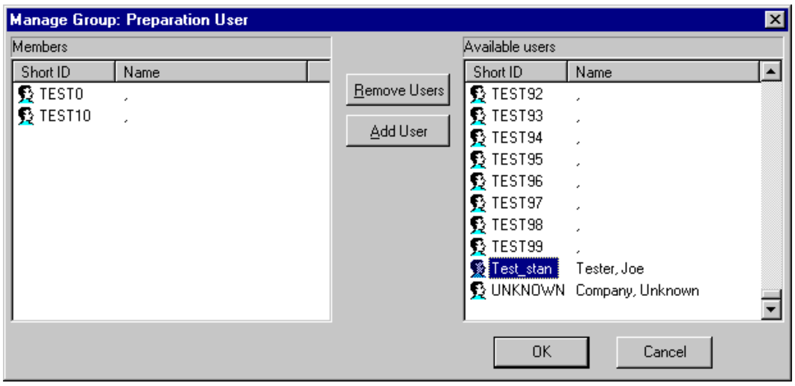
Adding a User to an Existing Group 12.8

When SampleTrack™ is first installed a default configuration of pre-defined groups is loaded in the Object Manager.

A user will automatically be added to the **All** group when the user is created in the Environment Setup of the SampleTrack™ client. If a user needs additional privileges, the first step is to determine if the access rights that they need are contained in an existing group. For example, if the new user needs access to reports that the Preparation User group uses, then they probably need to be added as a member to that group. If an existing group does not contain the necessary rights that a user needs, and you do not wish to add the rights that are lacking in an existing group, then you can create a new group for the user. There is no minimum requirement for the number of users that need to be in a group.

To add a user to a group, the user account must first be created in the **Environment Setup**. The user can then be inserted into a group by selecting the group with your mouse, and then selecting Edit - Manage Users, from the Object Manager main menu. This will open the group management tool for the group that you have selected. For example, if you click on the Preparation User group and open the management group tool the window shown below will appear.

Figure 12.8. Adding a New User (Or Group of Users)



Short ID	Name
TEST0	,
TEST10	,

Short ID	Name
TEST92	,
TEST93	,
TEST94	,
TEST95	,
TEST96	,
TEST97	,
TEST98	,
TEST99	,
Test_stan	Tester, Joe
UNKNOWN	Company, Unknown

To add a new user (or group of users) to the group you must only select the individual(s) from the available users list and press the **Add User** button. This will copy the user you have selected into the members side of the window. Likewise, to delete a user, select the user from the Members window and press the **Remove Users** button.

Example: Create a User Group

13

Creating a New Group 13.1

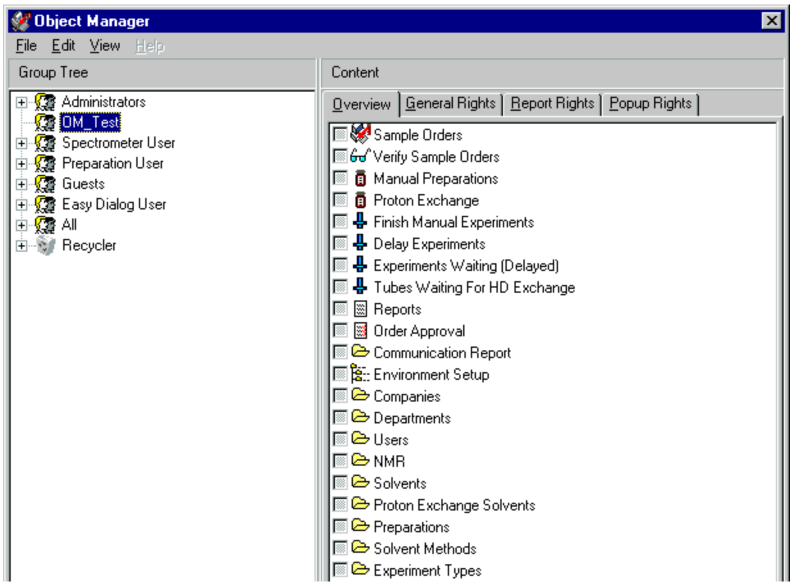
If you do not find a user in the list of available users, then the user has probably not been created in the Environment Setup.

If the available groups do not fit the requirements of a user you have the choice of modifying an existing group configuration, or adding a new group. The choice which is made really depends on your individual laboratory requirements. For example, it may not always be desirable to give an entire group access to a specific filter if only one person or a small number of the group require the filter. In this case the individual or small group can be granted access to the filter by creating a new group with this privilege. By also keeping them as members of the original group they maintain their current rights, but also have the new privilege.

Adding a Client Profile 13.2

The next step in adding a new group is to create a client profile. Select the new group that you have created. For an example I have created a group called OM_Test as shown in figure ***"Create a Client Profile" on page 105***. Select Edit - Insert Client Profile from the Object Manager main menu. A new Client Profile block will appear.

Figure 13.1. Create a Client Profile



The check boxes will all be shaded-gray when you first insert the new profile. You will need to go through each section of the Content window (Overview, General Rights, Report Rights and Popup Rights) and place a check mark in the box of the rights that you wish to assign to the new group. Likewise, if you want to disallow a right to a group, you will need to check the box so that the gray-shade disappears and a white box is displayed.

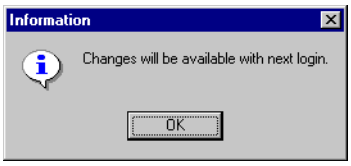
If a right has been assigned to the members of the group in a lower level (e.g. the **All** group) then you can leave the boxes gray-shaded.

When you finished making the appropriate selections, click anywhere in the group tree. You will be prompted as to whether you want to save the current client configuration, press **Yes** to save the new client profile (or **No** to exit without saving).

If you have saved the new client profile, the following window will be displayed, indicating that the changes (new client profile) will take place the next time you login to SampleTrack™:

You can continue to the next step of adding a new group without logging in. You should now see a new client profile under the new group that you have created in the **Group Tree** window.

Figure 13.2. Program Message



Changes will be available with next login.

Adding Table Defaults to the New Group *13.3*

The next step in adding a new client group is to add any required table default values that apply to the group. This tool is useful if the group repeatedly uses the same values in the Sample Orders, Methods, Preparations, or Experiment windows. By creating table defaults you can place the most often used values as the default value for a given field. For example, if the new group you have created uses the same project number in the Sample Order Details table (window) you can assign a default value to the project number.

To create a new table default value, select the group you want to add the table default to (click on the group with your mouse), and select Edit - Insert Table Defaults from the Object Manager main menu. A pop-up Edit Table Defaults window will appear as shown in the figure below:

Select a table from the pull-down menu **Table** that you wish to work with. As an example select the SAMPLE_ORDERS table, as shown in the following figure.

Figure 13.3. Adding Table Default Values for a Group

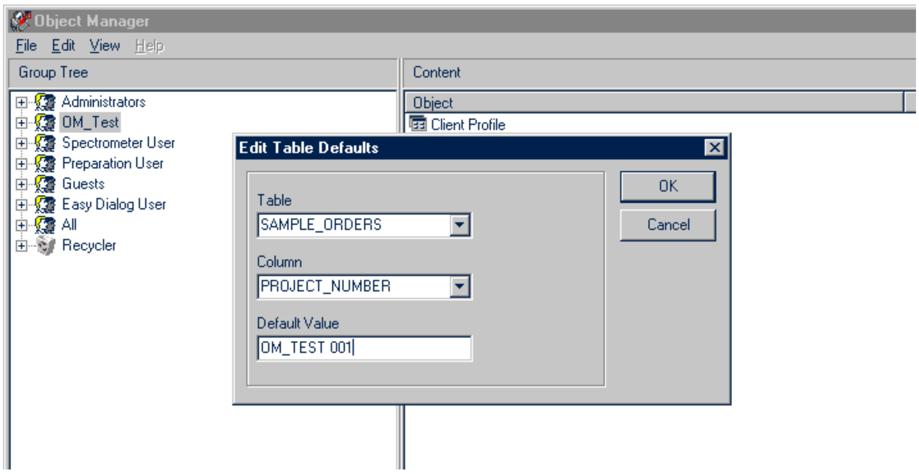


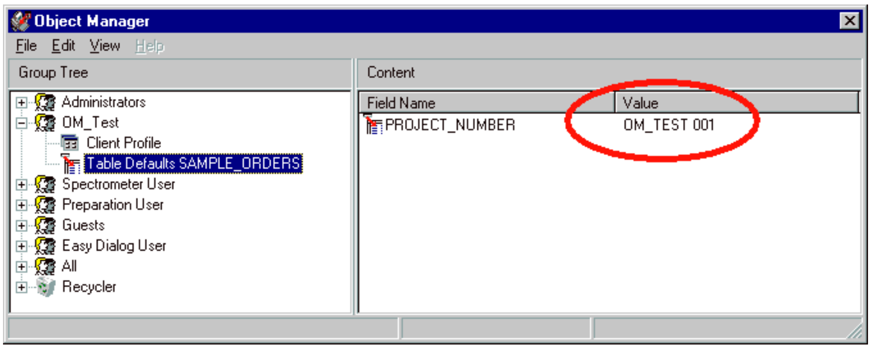
Table: SAMPLE_ORDERS

Column: PROJECT_NUMBER

Default Value: OM_TEST 001

Select the **PROJECT_NUMBER** field from the **Column** pull-down menu. Now enter the default value OM_TEST 001 in the **Default Value** input window. When you press the OK button the new table default value will be listed under your new group. To view this press the **+ Box** next to your group in the Group Tree, then click once on the new **Table Defaults SAMPLE_ORDERS** entry listed under the Client Profile. You should now see the OM_TEST 001 value listed under the Value column of the Content window as shown in the following figure:

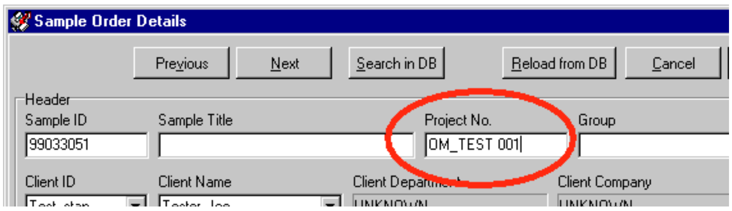
Figure 13.4. Defaults in the Content Window



Field Name	Value
PROJECT_NUMBER	OM_TEST 001

The next time that a user logs into this group, and makes an entry in the Sample Order Details window, the new default value will for example, appear in the Project Number field as shown below:

Figure 13.5. Example: Default Project Number



Sample ID: 99033051

Project No.: OM_TEST 001

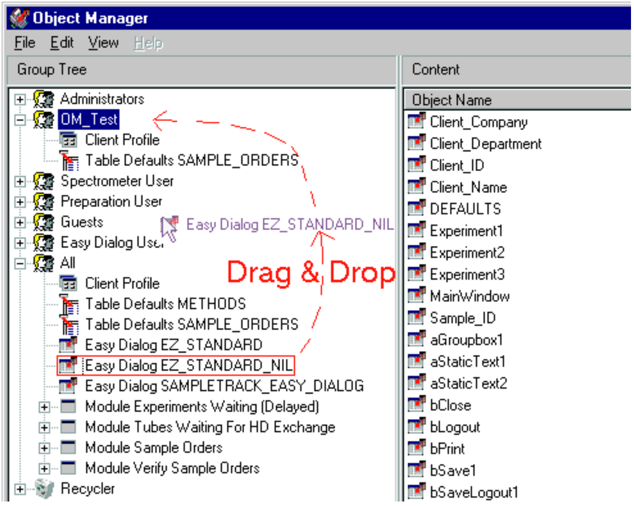
In the same manner the Project No. default value will appear in the group EasyDialog Window (if the Project No. field is used in EasyDialog).

The number of default values that can be used is unlimited, however it is only advisable to use these default table values when the value will normally be repetitive.

Inserting a New Group EasyDialog Configuration *13.4*

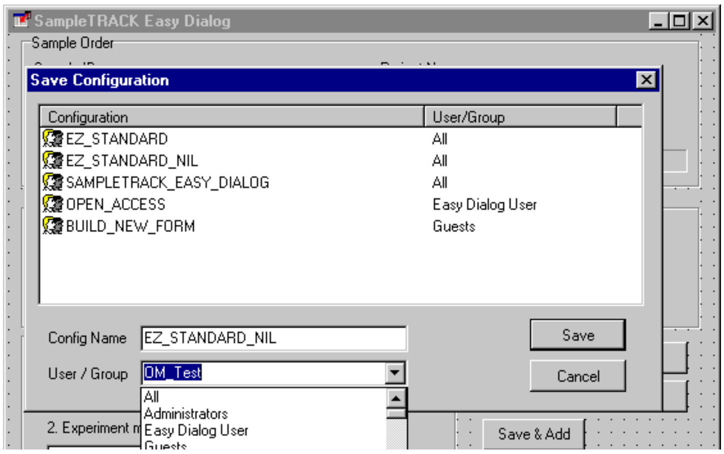
There are two methods available to assign an EasyDialog configuration to a user group. If an EasyDialog configuration already exists, such as the EZ_STANDARD shown in the following figure, you only need to drag & drop the configuration into your new group as illustrated below (or copy and paste if you prefer).

Figure 13.6. Drag and Drop EasyDialog Configuration to a Group



If an existing EasyDialog configuration does not fit the needs of the new user group that you have created, you can create a new EasyDialog configuration in the EasyDialog configuration tool and save it directly into the new group as illustrated in the next figure.

Figure 13.7. Save EasyDialog for a Specified User / Group



Configuration	User/Group
EZ_STANDARD	All
EZ_STANDARD_NIL	All
SAMPLETRACK_EASY_DIALOG	All
OPEN_ACCESS	Easy Dialog User
BUILD_NEW_FORM	Guests

Config Name: EZ_STANDARD_NIL

User / Group: OM_Test

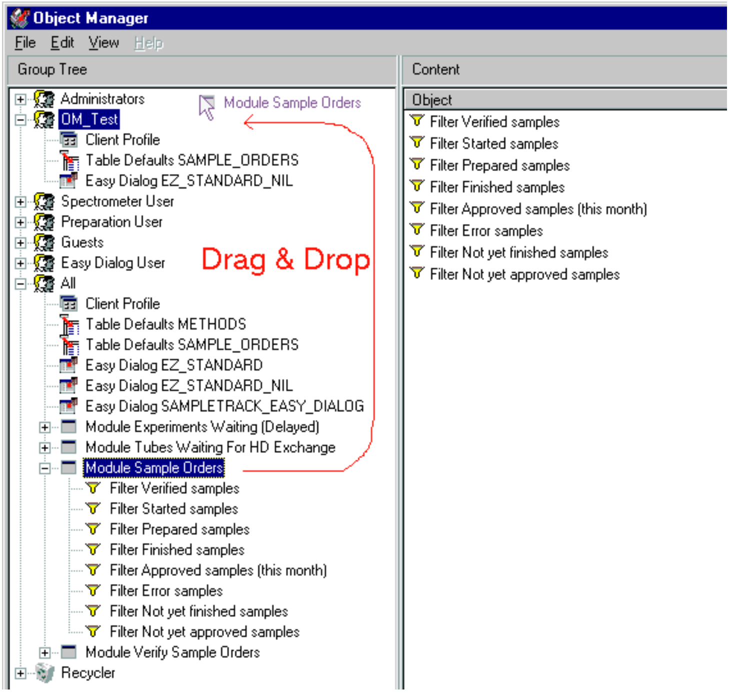
In either case a member of the group can then use this configuration when they log into EasyDialog.

Inserting a New Filter Method 13.5

In SampleTrack™, user specific filters can be stored under a user defined name and are available after each new log-in. In order to assign a new filter to a group, you must first select a module(s) for a group. The filter module is a group of related filters that are used for a specific activity, such as a sample order module, a module for experiments waiting etc.

If you want to apply the standard filters for Sample Orders, for example, you can drag & drop the Module Sample Order from the **All** group to your new group (see the figure below).

Figure 13.8. Drag and Drop Filter Configuration to a Group



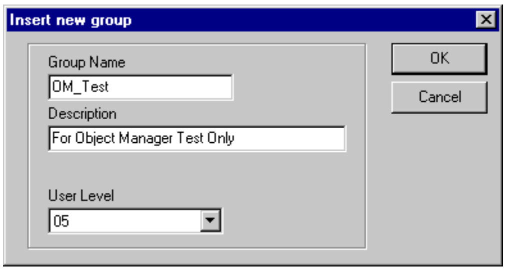
The group can then use the filters that accompany this group. You can add or delete existing filters to this module as needed. To create a new filter you must utilize the **Customize Filter Settings** in the SampleTrack™ Client Tool. Refer to the section **Filter & Search Tools** for details.

Inserting a New Group Name 13.6

To create a new group select Edit - Insert Group from the Object Manager main menu. An input window will appear asking for a new Group Name and Description, as shown in the figure below. By default the next available user level will be displayed in the User Level field. You can either use the default value, or select a different user level from the pull-down list. If you anticipate needing intermediate user levels in the future you should select a higher user level, e.g. 10. In any case you can change this user level at a later time as needed.

When you press OK, the new group will be added to the Group Tree.

Figure 13.9. User Level in the ***Insert New Group*** *Window*



Group Name
OM_Test
Description
For Object Manager Test Only
User Level
05

Handling the Tube ID

14

The Tube ID and TubeID.txt File 14.1

The Tube ID is the temporary identifier used to identify the sample after the preparation during the NMR measurement. This Tube ID is part of the NMR method table of each sample order and is entered either manually by the preparer or during the communication, e.g.with the NMR B-ACS system.

The TubeID.txt file contains a list of all Tube ID's in use.

Automatic Entering of the Tube ID 14.2

During the sample preparation performed by the NMR B-ACS, the barcode collar with the associated Tube ID is taken at random from the collar dispensing station. If the NMR B-ACS receives a collar with a barcode already in use, the collar is rejected and a new one will be taken from the dispensing station. The Tube ID number is then recorded by NMR B-ACS in the preparation report file.

During the file import by the SampleTrack™ software import module, the sample Tube ID is entered in the method table of the associated data set in the Oracle® database, and the TubeID.txt file is updated.

Entering the Tube ID Manually 14.3

During the manual preparation of an order, the preparer must manually enter the Tube ID number.

Updating the Jobs in the Tube ID File 14.4

The Tube ID file is updated through the triggering of the SampleTrack™ communication server by the database, which results in the scanning of all the orders in the database. The Tube ID's of all orders with header status equal or greater than **Started** and below **Approved** are written to the file.

Through this process a Tube ID of a deleted or approved order is removed from the file and can be reused.

System Parameters

15

SampleTrack™ Client Parameters 15.1

/MultiInstance:	Allows more than one instance from SampleTrack™ Client to be opened.
/Username:<usr>:	The login user name: e.g. GUEST
/Password:<Passwrd>:	Password for a corresponding user.
Example 1:	C:\Programs\Bruker\SampleTrack\bin\STClient.exe /UserName:JOE /Password:test
Example 2:	C:\Programme\Bruker\SampleTrack\bin\STClient.exe /Multiinstance /Username:admin /Password:mypassword

EasyDialog Parameters 15.2

/Username:<usr>:	The login user name: e.g. GUEST
/Password:<Passwrd>:	Password for a corresponding user.
/Admin:	The program will be opened in EasyDialog configuration mode (the Toolbars appear).
/Config:	EasyDialog is opened with the Load Configuration window to allow EasyDialog configuration selection.
/Config:<Name>:	EasyDialog is opened with the <name> as a parameter. When this name does not exist the program will be halted.
/SysButtons:	Displays the system Windows button and system menu when EasyDialog is opened.

Shortcuts in SampleTrack™

16

The following shortcuts are used in most SampleTRACK windows. Some of them are not yet implemented.

Ctrl-A	Select all
Ctrl-C	Copy content
Ctrl-D	Delete method
Ctrl-F	Search
Ctrl-I	Version Info
Ctrl-O	Start Object Manager
Ctrl-P	Print screenshot
Ctrl-R	Start DB Registry Editor
Ctrl-V	Paste content
Ctrl-X	Cut content

F1	Help
F3	Continue search
F5	Refresh
F6	New record
F7	Copy record
F8	Save to database
F9	Submit
F12	Superuser Mode on / off

SampleTrack™ Tables

17

SampleTrack™ Base Tables 17.1

Introduction to SampleTrack Base Tables 17.1.1

The base tables are used internally by both EasyDialog and the Object Manager. When using database version V2.033 there are four base tables used to setup a sample order:

SAMPLE_ORDERS (header information)

METHODS (method specific header information, e.g. NMR, MS, IR ...)

NMR_PREPARATION_WS (NMR preparation information)

NMR_EXPERIMENT_WS (NMR experiment information)

The base tables are linked via primary and foreign keys as illustrated below:

```
SAMPLE_ORDERS
| ------> METHOD (NMR)
| ------> NMR_PREPARATION_WS
                    | ------>NMR_EXPERIMENT_WS
```

The Fields Overview section of the EasyDialog configuration window contains these very same tables and fields:

The EasyDialog Fields Overview 17.1.2

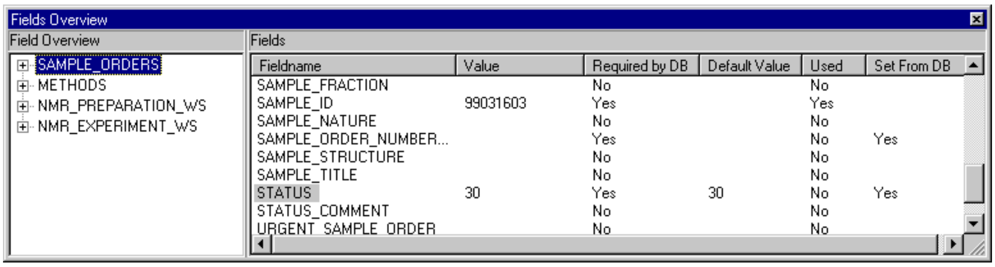
Refer to the chapter on EasyDialog specific help for details on the selection and use of the individual fields. see also: ***"The Fields Overview Window" on page 127***

The tables that follow describe the meaning of each field found in the base tables.

The **Field** column in each table represents the name of the field as it appears in SampleTrack™ (e.g. in the EasyDialog Fields Manager).

Likewise the **Description** column is a short explanation of what the field is.

Figure 17.1. Field Overview



Fieldname	Value	Required by DB	Default Value	Used	Set From DB
SAMPLE_FRACTION		No		No	
SAMPLE_ID	99031603	Yes		Yes	
SAMPLE_NATURE		No		No	
SAMPLE_ORDER_NUMBER...		Yes		No	Yes
SAMPLE_STRUCTURE		No		No	
SAMPLE_TITLE		No		No	
STATUS	30	Yes	30	No	Yes
STATUS_COMMENT		No		No	
URGENT_SAMPLE_ORDER		No		No	

The SAMPLE_ORDER Table *17.1.3*

Field	**Description**
Sample_Order_Number_Key	The unique, internal number used as the primary key for the SampleTrack™ SAMPLE_ORDERS table.
Sample_ID	The unique sample ID used for the sample in SampleTrack™.
Sample_Title	Free entry (could be used for the plot title in older versions).
Sample_Nature	Free entry.
Sample_Charge	Free entry.
Sample_Fraction	Free entry.
Project_Number	Free entry.
Date_Entry	Date when the record was created.
Date_Start	Date when the sample preparation was started.
Date_End	Date when the last experiment was finished.
Status	The status of the sample. The following status are available:
	10 Created
	20 Verified
	30 Started
	40 Working
	50 Pause
	60 Finished
	70 Approved

	80 Archived
	95 Instrument error
User_Name_Key	The SampleTrack™ Client ID abbreviation (a required field).

The METHODS Table 17.1.4

Field	Description
Sample_Order_Number_Key	The foreign key used for the sample orders table.
Method_Type_Key	The method type (currently only NMR).
Plot_Title	The title for the spectra plot.
Journal_Number	The journal number field.
Sample_Changer_Holder	The last position of a tube in the sample changer holder.

The NMR_PREPARATION_WS Table 17.1.5

Field	Description
NMR_Preparation_WS_Key	The unique, internal number used as the primary key for the SampleTrack™ NMR_PREPARATION_WS table.
Sample_Order_Number_Key	The foreign key used for the methods table, used in conjunction with the Method_Type_Key.
Method_Type_Key	The foreign key used for the methods table, used in conjunction with the Sample_Order_Number_Key.
Sample_Amount	The quantity of the sample being used.
Solvent_Amount	The quantity of the solvent being used.
Solvent_Name_Key	The solvent name used in the SampleTrack™ preparation (a required field).
Instrument_Name_Key	The instrument name used in the SampleTrack™ preparation (a required field).
Preparation_Name_Key	The preparation name used in the SampleTrack™ preparation (a required field).
User_Name_Key	The user who has prepared the sample.
Date_End	The date when the preparation was finished.
Status	The status of the preparation. Refer to the available status in the SAMPLE_ORDERS table

The Experiment Table 17.1.6

Field	Description
NMR_Experiment_WS_Key	The unique, internal number used as the primary key for the SampleTrack™ NMR_EXPERIMENT_WS table.
NMR_Preparation_WS_Key	The foreign key used for the NMR_PREPARATION table.
Experiment_Name_Key	The unique name of the SampleTrack™ experiment (also composite).
Composit_Experiment	The name of the sub-experiment.
Experiment_Type_Name_Key	The type of experiment (1H, C12...).
Experiment_ID	The ID used for each experiment.
Instrument_Name_Key	The instrument name used in the SampleTrack™ experiment (a required field).
Result_Data_Path	The local path for the instrument data results.
User_Name_Key	The user who has performed the experiment.
Date_Start	The date the experiment was started.
Date_End	The date when the experiment was finished.
Status	The status of the experiment Refer to the available status in the SAMPLE_ORDERS table

VCU Request Tables 17.2

Introduction to VCU REQUEST Tables 17.2.1

The VCU_REQUEST_ALL view is utilized when you desire to compile statistical or report data to view with an external program such as Crystal Reports™ or Microsoft® Excel®. For example, you can compile a report in Microsoft® Excel® that shows all of the Proton experiments that have been completed.

A basic understanding of ODBC, SQL and tables is assumed when working with external programs. Refer to your external program handbook for assistance.

The fields that are listed in the following tables will assist you in configuring a link from your external program (using e.g. ODBC or SQL) to various data in SampleTrack™.

The VCU Sample Order Table 17.2.2

Field	Description
User_Name_Key	The client short ID, must exist in SampleTrack™.
Last_Name	Last name of the client.

First_Name	First name of the client.
Department_Name_Key	Department name, must exist in SampleTrack™.
Sample_ID	The unique sample ID used for the sample in SampleTrack™.
Sample_Title	Free entry (could be used for the plot title in older versions).
Sample_Nature	Free entry.
Sample_Charge	Free entry.
Sample_Fraction	Free entry.
Project_Number	Free entry.
Date_Entry	Date when the record was created.
Date_Start	Date when the sample preparation was started.
Date_End	Date when the last experiment was finished.
Status	The status of the sample. The following status are available: 10 Created 20 Verified 30 Started 40 Working 50 Pause 60 Finished 70 Approved 80 Archived 95 Instrument error

The VCU Preparation Table *17.2.3*

Field	**Description**
Method_Type_Key	Method Type (only NMR in the moment).
Plot_Title	Title for the plot of the spectra.
Sample_Amount	Amount of the sample used.
Solvent_Name_Key	Solvent name for the preparation, must exist in SampleTrack™.
Instrument_Name_Key	The instrument name used for the preparation, must exist in SampleTrack™.
Preparation_Name_Key	The name of the preparation, must exist in SampleTrack™.
User_Name_Key_1	User who started the preparation.
Date_Start_1	Date when the preparation was started.
Date_End_1	Date when the preparation was finished.

Status_1	Status of the preparation. The status could be the same as one of the above.

The Experiment Table (VCU_REQUEST_ALL) *17.2.4*

Field	Description
Composit_Experiment	The name of the sub-experiment.
Experiment_Name_Key	The unique name of the SampleTrack™ experiment (also composite).
Experiment_Type_Name_Key	The type of experiment (1H, C12...).
Experiment_ID	The ID used for each experiment.
Instrument_Name_Key_1	The instrument name used in the SampleTrack™ experiment (a required field).
Result_Data_Path	The local path for the instrument data results.
User_Name_Key_2	The user who has performed the experiment.
Date_Start_2	The date the experiment was started.
Date_End_2	The date when the preparation was finished.
Status_2	The status of the experiment. The status could be the same as one of the above.

EasyDialog Configuration

18

Opening the EasyDialog Configuration Window 18.1

You will need to have administrator privileges to perform the EasyDialog configuration. To open the EasyDialog designer open the Administration pull-down menu and select: *Start EasyDialog Designer*

Figure 18.1. The Start EasyDialog Designer Menu Option

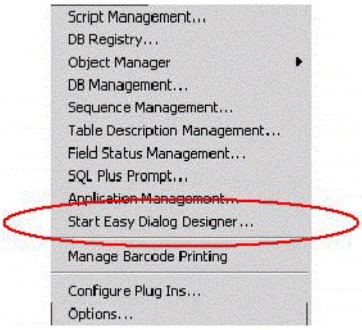
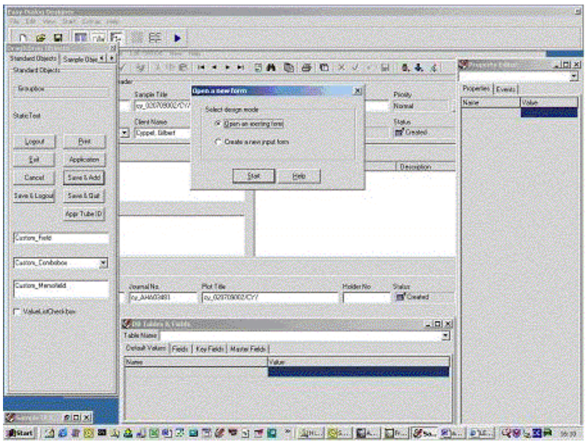


Figure 18.2. The EasyDialog Configuration Overview Window



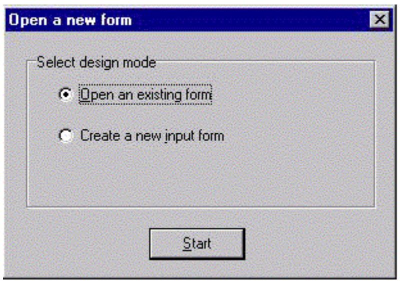
Opening a Form / Creating a New Form 18.2

The configuration of EasyDialog is accomplished through a object-oriented, drag, drop & modify methodology. To prepare a user input or request form you must only select an object from a list, drag it onto a design screen, and edit the specific parameters for that object. By selecting various pre-programmed object modules in this manner you can adjust the form to fit the individual needs of your user or group of users.

There are currently two modes in the EasyDialog configuration window: Open an Existing Form or Create a New Input Form.

Upon entering the configuration window you will be presented with the following window where you can select the design mode that you wish to use:

Figure 18.3. Open / Create a New Form



If you wish to open an existing form to revise or to use as a template select Open an Existing Form. You will then be able to modify the form, and to save the changes that you make to the form as the original form name, or under a new name.

If you wish to create an entirely new input form, select Create a New Input Form.

Note: An input form is a form (or input screen) where a user supplies information, for example, for a preparation or an experiment that they want to perform.

The Configuration Window *18.3*

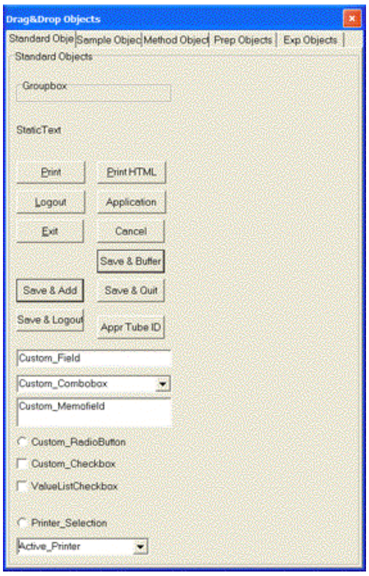
There are five main panels which make up the EasyDialog Configuration Tool:

- The Administrator Toolbar
- The Drag & Drop Objects
- The Property Editor
- The Fields Overview
- The new form itself

Drag & Drop Objects *18.4*

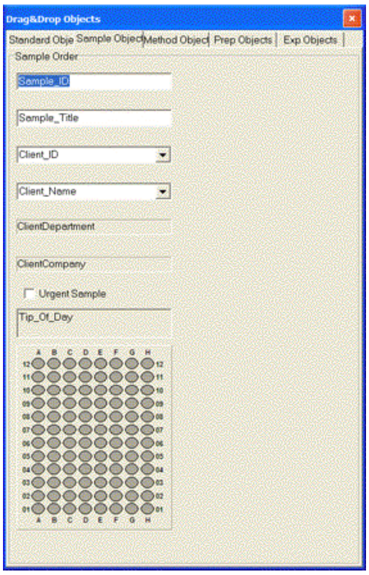
The Drag & Drop Objects window consists of a collection of pre-defined objects. These objects can then be used to build new input forms.

Figure 18.4. Drag & Drop Objects



The objects are seperated systematically within Tab windows, grouping standard objects like ‘printer selection’, ‘Save’ buttons or custom fields, custom combo boxes, check boxes or radio buttons, that are not defined in the standard database fields.

Figure 18.5. The Drag & Drop Objects Window

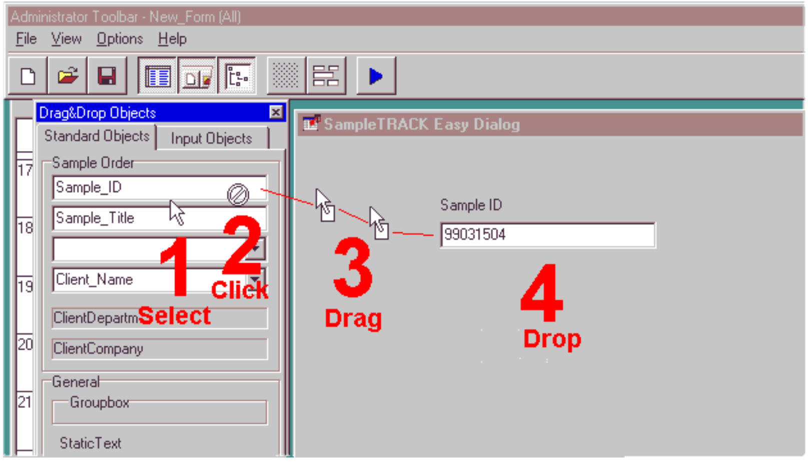


The fields in the sample order, method ,preparation and experiment tabs are typical fields used in an adapted EasyDialog form. Custom fields are saved in the database in the same manner as the standard fields.

How to Drag & Drop Objects 18.5

This object-oriented programming approach to form building, allows a non-programmer to quickly and easily build new EasyDialog forms. To use these objects in a new form you must only select one, click once on the object with your left mouse button and hold the button down while you drag the object onto your new form. The figure below illustrates this simple drag and drop process.

Figure 18.6. Drag - Drop Objects



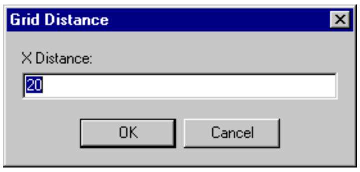
Sample ID: 99031504

Grids 18.6

In order to simplify the alignment of the objects in the new form, a grid system has been implemented. By enabling the grid (Options - Grid - Enable Grid) you can align the new objects on the X and Y coordinates of the grid lines.

The distance between the grid lines is adjustable. To change the grid distance select Options - Grid - Change X or Change Y Grid Distance. An input window will appear which will allow you to enter the new grid distance:

Figure 18.7. Changing the Grid Distance

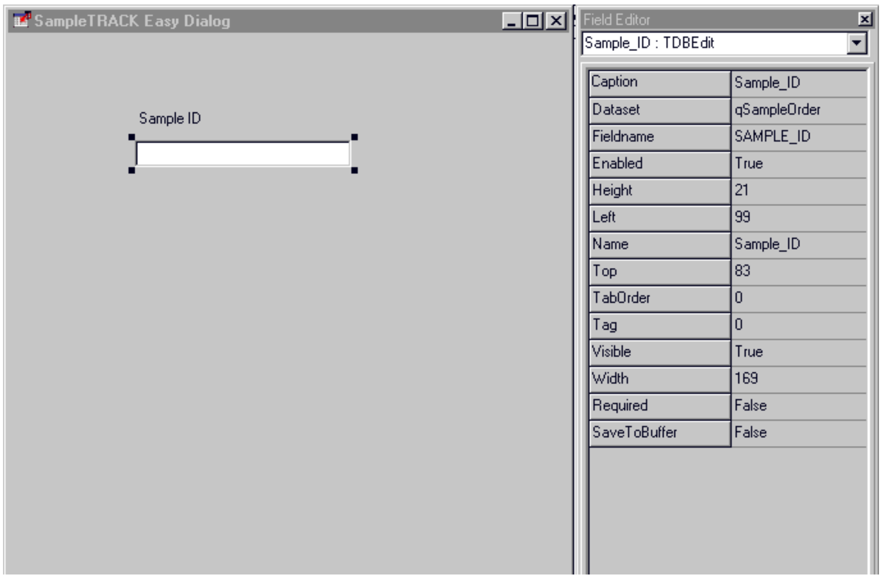


X Distance: 20

The Property Editor 18.7

Once an object has been dropped into a new form you can configure the object field or title using the Property Editor. To configure a new object, click on the object in the new form with your mouse. The Property Editor will display the current attributes of the object. You can then make any changes to these attributes as needed. When you have several objects on your form you must only click on the corresponding object to change its attributes.

Figure 18.8. Configuring a New Object for EasyDialog



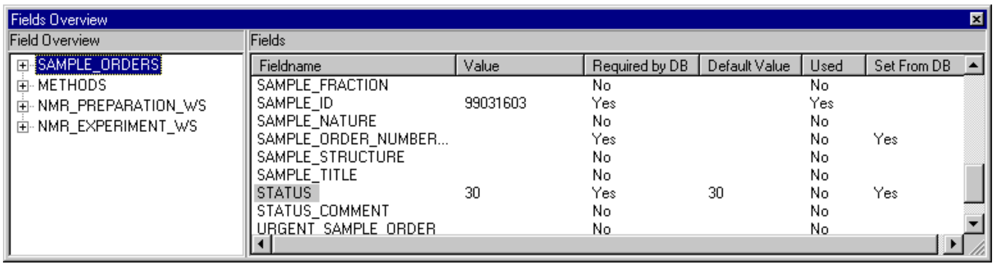
Sample_ID : TDBEdit

Caption	Sample_ID
Dataset	qSampleOrder
Fieldname	SAMPLE_ID
Enabled	True
Height	21
Left	99
Name	Sample_ID
Top	83
TabOrder	0
Tag	0
Visible	True
Width	169
Required	False
SaveToBuffer	False

The Fields Overview Window 18.8

The Fields Overview window is a second source of objects for your new form. The fields listed here are the actual fields that are found in the SampleTrack™ database. Normally these should only be used if an object is not found in the Drag & Drop Objects, or if a special definition is required.

Figure 18.9. The Field Overview Window



Fieldname	Value	Required by DB	Default Value	Used	Set From DB
SAMPLE_FRACTION		No		No	
SAMPLE_ID	99031603	Yes		Yes	
SAMPLE_NATURE		No		No	
SAMPLE_ORDER_NUMBER...		Yes		No	Yes
SAMPLE_STRUCTURE		No		No	
SAMPLE_TITLE		No		No	
STATUS	30	Yes	30	No	Yes
STATUS_COMMENT		No		No	
URGENT_SAMPLE_ORDER		No		No	

The Fields Overview window in the example is broken down into four main sections: SAMPLE_ORDERS, METHODS, NMR_PREPARATION_WS, and NMR_EXPERIMENTS_WS. Each section has several corresponding fields, as shown in the Fields box in the figure above, which can be dragged & dropped onto a form.

The SAMPLE_ORDERS fields represent the main information that will be included in EasyDialog. The METHODS section contains the fields that pertain specifically to methods. Likewise, NMR_PREPARATION_WS and NMR_EXPERIMENTS_WS contain fields that pertain specifically to worksteps for preparations and experiments, respectively.

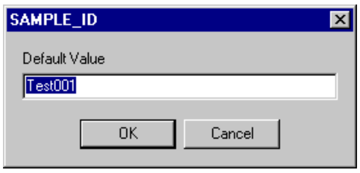
Fields Overview Required Values *18.9*

Certain fields are required by the database, and are identified with a **Yes** in the **Required by DB** column. When a field is required by the database, then a value must be provided. This value can be derived from three sources. The first is that the value is set by the database automatically. In this case the **Set From DB** column will contain a **Yes** value. The second method is to define a default value for the field (see ***"Default Values in the Fields Overview Window" on page 128***). If the value is not derived from the first two methods, then the field must be present in the EasyDialog form so that the user can enter this value.

Default Values in the Fields Overview Window *18.10*

When you double-click with your mouse on one of the fields, a window will appear that will allow you to enter a default value to the corresponding field:

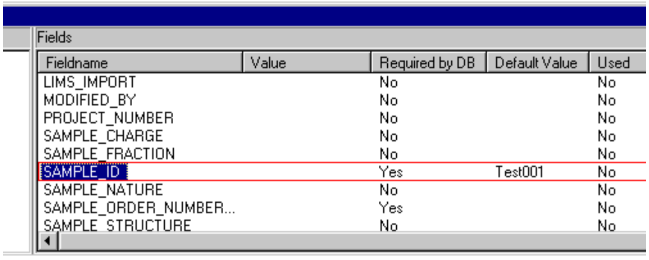
Figure 18.10.Default Field Value in the Fields Overview Window



Default Value: Test001

The default value is then displayed in the **Default Value** column of the Fields Overview window.

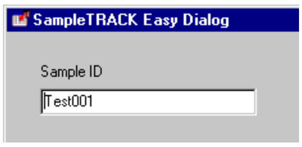
Figure 18.11.Default Value in the Fields Overview Window



Fieldname	Value	Required by DB	Default Value	Used
LIMS_IMPORT		No		No
MODIFIED_BY		No		No
PROJECT_NUMBER		No		No
SAMPLE_CHARGE		No		No
SAMPLE_FRACTION		No		No
SAMPLE_ID		Yes	Test001	No
SAMPLE_NATURE		No		No
SAMPLE_ORDER_NUMBER...		Yes		No
SAMPLE_STRUCTURE		No		No

This default value will then be displayed when you start EasyDialog.

Figure 18.12.Default Value in EasyDialog



Sample ID: Test001

The STATUS Field *18.11*

There are several pre-defined status entries used by SampleTrack™. The table below lists the current status codes and their meaning:

Status Code	Description
10	Created
20	Verified
25	Waiting
30	Started
60	Finished
70	Approved

In the Fields Overview window, the SAMPLE_ORDERS, the NMR_PREPARATION_WS, and the NMR_EXPERIMENTS_WS categories each contain a STATUS field. By using this STATUS field you can assign a default status code value to each category from the table above.

The point at which a Sample Order, Preparation or Experiment is assigned one of these status‘s is completely definable by the administrator in the EasyDialog configuration. For example, in one laboratory setup, the user might bring the sample to the laboratory where further preparations will be carried out, and the responsible laboratory personnel will place the sample on the sample changer. In this system the user‘s EasyDialog should set the Sample Order to status „Created“ or „Verified“ when the user presses OK. The laboratory personnel would then use the Verify Sample Orders or Manual Preparations windows in the Client Tool to upgrade the status‘s when the preparation has been completed.

In an open access system, for example, where the user has access to a spectrometer and can place the samples that they have prepared on the sample changer themselves, EasyDialog must be configured so that the user can manually enter a Tube ID and Sample ID. In this case, when the user presses the OK button in EasyDialog, the Sample Order status should be set to „Started“, the Preparation status to „Finished“, and the Experiment status to „Verified“.

There are of course many different versions of these scenarios that could be used in a laboratory. EasyDialog can be configured for your individual laboratory situation.

In any case the method used to configure which status will be achieved at what point, is completely programmable by the administrator in the EasyDialog configuration.

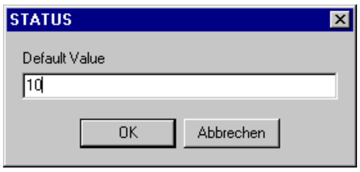
Configuring a Status *18.12*

To configure the status of the Sample Order, Preparation or Experiment, double-click with your mouse on the „Status“ field located in the Fields Overview panel under SAMPLE_ORDER, NMR_PREPARATION_WS, or NMR_EXPERIMENT_WS, respectively.

A default value window will appear (see the figure below) where you can place one of the status codes. For example, to set the Sample Order to **10** where it will be placed on status **Created**, when the user clicks the OK button in EasyDialog. Double click with your mouse on the **Status** field under SAMPLE_ORDER in the

Fields Overview window. When the default value window appears enter the status code for **Created**, which is **10** in the input box, as shown in the figure below.

Figure 18.13.Entering a Default Status Value



STATUS

Default Value: 10

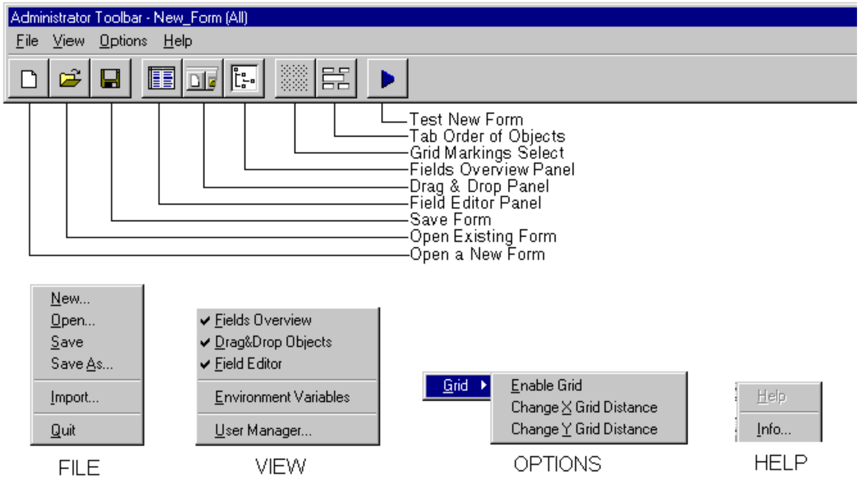
Press the **OK** button in the default value window to accept this new value. You should now see your new default value listed under the default value for SAMPLE_ORDER - Status in the Fields Overview window.

You can likewise set a default value listed in the Sample Status Code table to the preparation status and experiment status in this manner.

The Administrator Toolbar *18.13*

The Administrator Toolbar consists of a pull-down menu and several buttons which allow you to select various routine (e.g. Open, Save) and specialized tasks or options (e.g. environment variables, grid settings). You can also choose which panels are displayed, by (de)selecting the corresponding button from the button bar.

Figure 18.14.The Administrator Toolbar



Example: Creating a New Input Form *18.14*

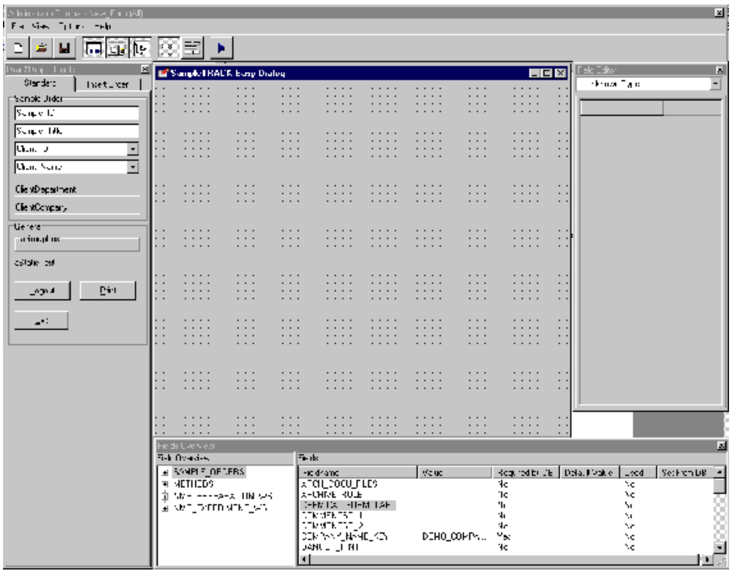
The following form example provides a detailed step-by-step description of how to build a new input form. If you have not already done so, read the help section ***"Opening a Form / Creating a New Form" on page 123*** to select a design mode before proceeding with this example.

Creating a New Form: Opening the Form 18.14.1

To create a new form select Create a New Input Form from the opening prompt, or File - New from the EasyDialog menu, then Create a New Input Form.

A new form will appear, similar to the one in the following figure:

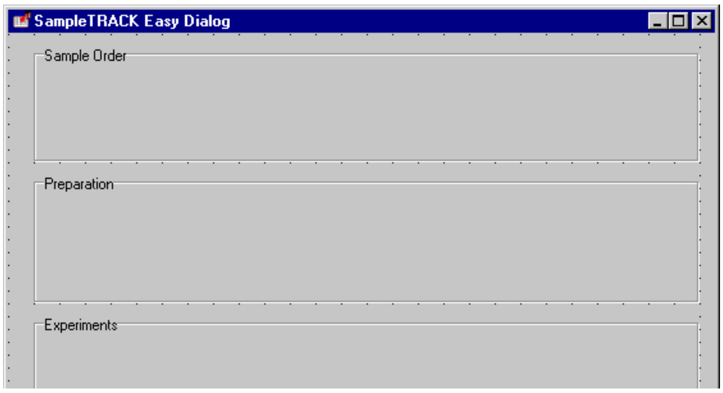
Figure 18.15.A New Input Form



Creating a New Form: Establishing Group Boxes 18.14.2

In creating the outline of a new form it is normally a good design methodology to first establish certain input areas which group related fields. This is accomplished most easily by using a „Group Box“. In our example here I will use Sample Order, Preparation and Experiments. Drag three group boxes from the Drag & Drop Objects window onto you new form. Fill-in the title for each group box by clicking once on the box to select it, and by filling in the Caption block of the Field Editor. When you have completed these steps your form should look something like the following figure.

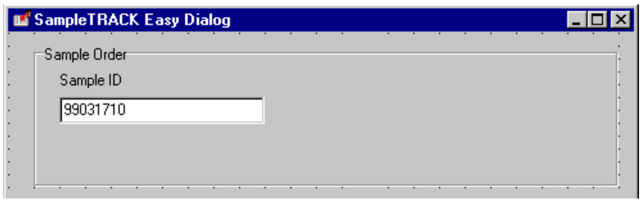
Figure 18.16.Drag and Drop Group Boxes



Creating a New Form: Adding the First Object 18.14.3

Drag & drop a Sample_ID object from the Drag & Drop Objects onto the Sample Order group box.

Figure 18.17.Drag and Drop Field Sample ID

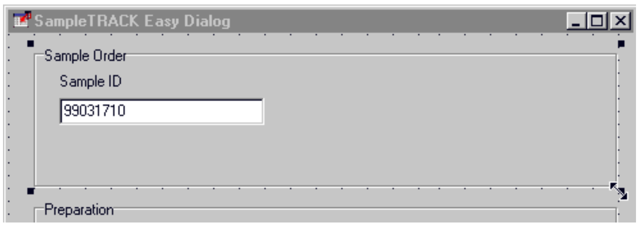


Sample ID
99031710

Don’t be alarmed if the object doesn’t fit properly, you can adjust the size of the Sample Order group box by clicking once on the group box to highlight it, then by pulling on one of the highlighted corners to adjust the size; or by changing the respective values (Left, Top, Width, and Height) in the Fields Object window.

Creating a New Form: Adjusting the Group Box 18.14.4

Figure 18.18.Adjusting the Size of an Object



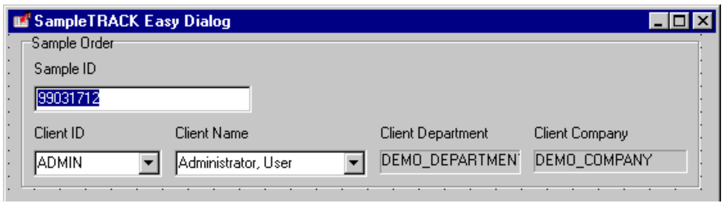
Sample ID
99031710

You can also adjust the size of an object in the same manner as described above.

To continue with our example, add the following objects to your Sample Order group box: Client_ID, Client_Name, Client_Department and Client_Company. Adjust the size of the objects and group box until they similar to those shown in the figure below. If you desire a Client Department and Client Company title, drag & drop two StaticText objects to the Sample Order group box and fill in the appropriate Caption in the Field Editor.

Creating a New Form: The Completed Group Box 18.14.5

Figure 18.19.The complete Group Box



Sample ID
99031712

Client ID
ADMIN

Client Name
Administrator, User

Client Department
DEMO_DEPARTMEN

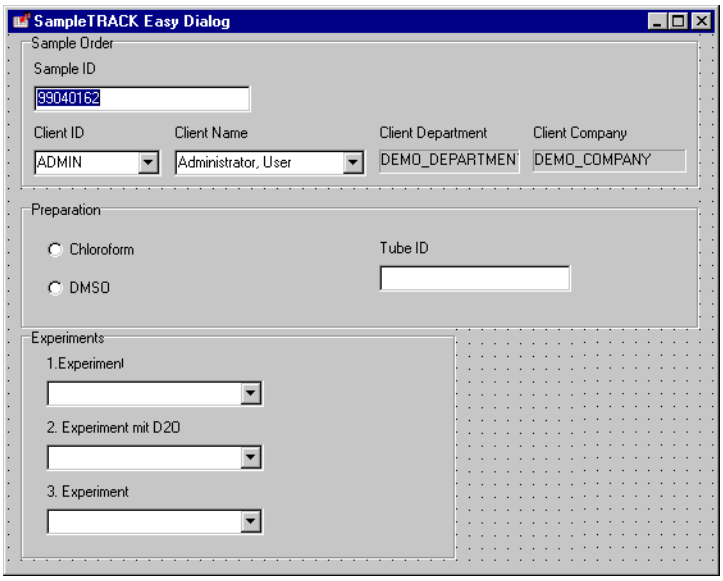
Client Company
DEMO_COMPANY

You will notice that the values (ADMIN, Administrator, User, DEMO_DEPARTMENT and DEMO_COMPANY) that are shown in the figure above are not in the field objects that you have entered. These will appear the first time you run this new form. The values represent the internal field values from the SampleTrack™ database.

Creating a New Form: Adding the Other Group Boxes *18.14.6*

Now fill in the fields as described previously until the Preparation and Experiment group boxes are completed as shown in the following figure:

Figure 18.20.Adding Group Boxes



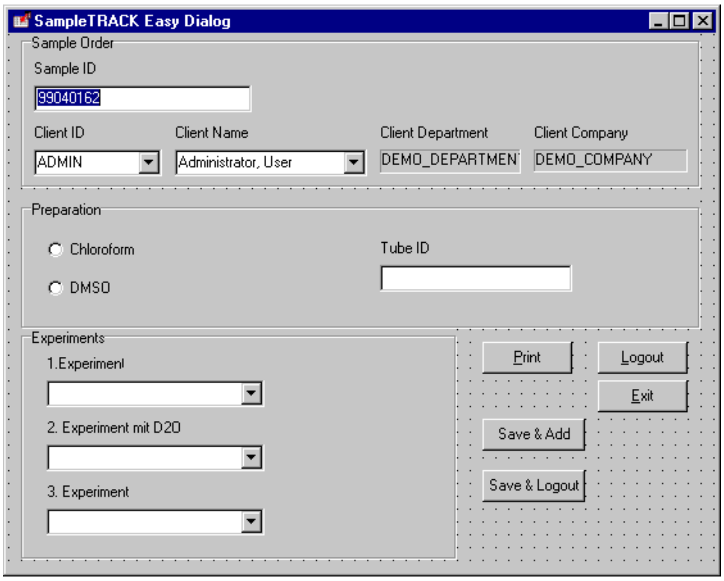
Sample ID: 99040162
Client ID: ADMIN
Client Name: Administrator, User
Client Department: DEMO_DEPARTMEN
Client Company: DEMO_COMPANY

Creating a New Form: Adding Buttons *18.14.7*

The final configuration features that needs to be added to complete our example are the task buttons. The Static Text buttons are pre-defined and configurable, you need only to drag and drop the objects onto your new EasyDialog form and adjust the parameters in the Field Editor. The exact buttons that you use depend on the tasks that you want the user to perform.

In the following example I have added some of the normal buttons that are used in EasyDialog.

Figure 18.21.Adding Buttons in a Form



Sample ID: 99040162

Client ID	Client Name	Client Department	Client Company
ADMIN	Administrator, User	DEMO_DEPARTMEN	DEMO_COMPANY

○ Chloroform

○ DMSO

Tube ID

1.Experiment

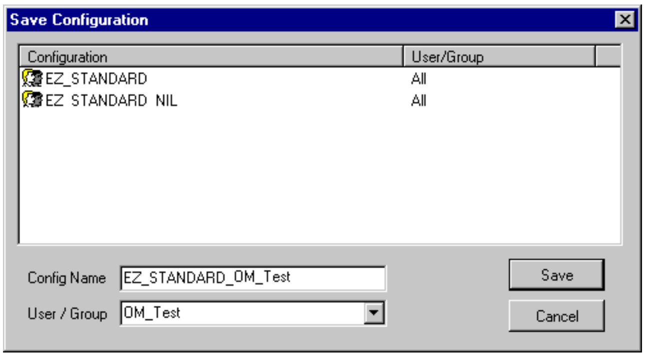
2. Experiment mit D2O

3. Experiment

Saving an EasyDialog Configuration 18.14.8

To complete the EasyDialog form select File - Save As from the EasyDialog main menu. A „Save As“ window will appear, as shown in the following figure, that will prompt you for a Configuration Name and User/Group under which to save the ile.

Figure 18.22.Save EasyDialog configuration



Configuration	User/Group
EZ_STANDARD	All
EZ_STANDARD_NIL	All

Config Name: EZ_STANDARD_OM_Test

User / Group: OM_Test

Enter a configuration name such as EZ_STANDARD_<new name>, where <new name> is a name that you give the file. If you want to save the configuration under an existing name (e.g. EZ_STANDARD), select the name from the configuration list - this will overwrite the existing file.

For the User/Group select a group or user from the pull-down menu. If you want to make the new EasyDialog configuration available for all users, select „All“, otherwise select the specific user or group that you want the configuration assigned to.

This completes the steps for creating a new form.

EasyDialog Parameters *18.15*

/Username:<usr>: The login user name: e.g. GUEST

/Password:<Passwrd>: Password for a corresponding user.

/Admin: The program will be opened in EasyDialog configuration mode (the Toolbars appear).

/Config: EasyDialog is opened with the Load Configuration window to allow EasyDialog configuration selection.

/Config:<Name>: EasyDialog is opened with the <name> as a parameter. When this name does not exist the program will be stopped.

/SysButtons: Displays the system Windows button and system menu when EasyDialog is opened.

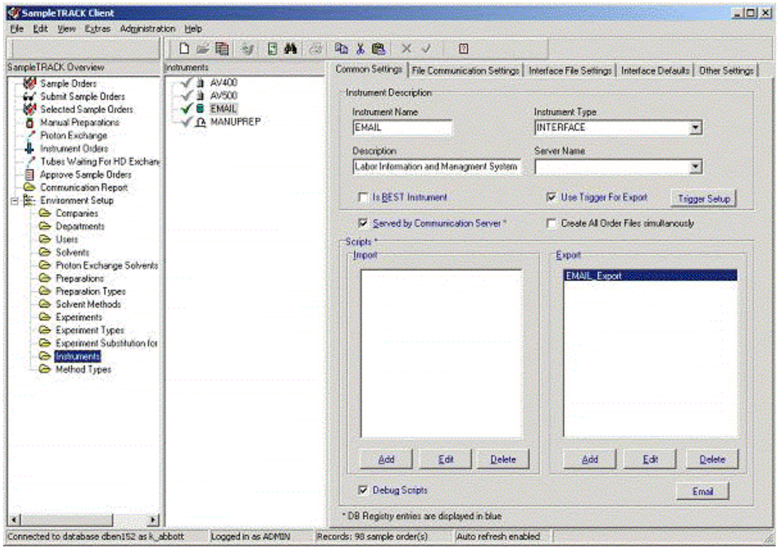
E-Mail Support 19

E-Mail Support 19.1

An additional feature of SampleTrack is the ability to notify users of finished samples or experiments per E-mail. In order to notify users per E-mail, the E-mail addresses must first be added to the E-mail listing in the Environment Setup – Users – Basic Information window. New users can either be inserted manually or through file import.

The generation of E-mails is executed by the database and the SampleTrack Communication Server. The Communication Server handles E-mail support like an instrument, no user interaction is necessary. To activate E-mail notification, check **Served By Communication Server** in the **Envoronment Setup / Instruments / E-mail** window.

Figure 19.1. E-mail Served by the Communication Server



Instrument Description

Instrument Name: EMAIL

Instrument Type: INTERFACE

Description: Labor Information and Managment System

Server Name:

☐ Is BEST Instrument

☑ Use Trigger For Export

☑ Served by Communication Server *

☐ Create All Order Files simultanously

Scripts *

Import:

Export: EMAIL_Export

☑ Debug Scripts

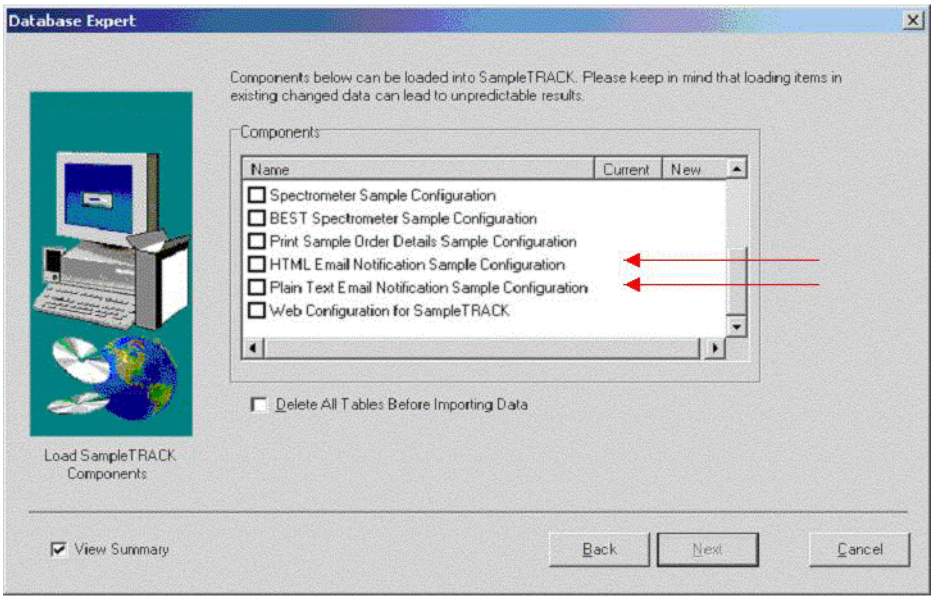
* DB Registry entries are displayed in blue

Connected to database dben152 as k_abbott | Logged in as ADMIN | Records: 98 sample order(s) | Auto refresh enabled

Installation of E-mail support 19.2

Start the installation in the **Administration** menu, **DB Management** / **Load Components**.

Figure 19.2. Selecting HTML or Plain Text E-mail Notification



Components below can be loaded into SampleTRACK. Please keep in mind that loading items in existing changed data can lead to unpredictable results.

☐ Spectrometer Sample Configuration
☐ BEST Spectrometer Sample Configuration
☐ Print Sample Order Details Sample Configuration
☐ HTML Email Notification Sample Configuration
☐ Plain Text Email Notification Sample Configuration
☐ Web Configuration for SampleTRACK

☐ Delete All Tables Before Importing Data

☑ View Summary

Installation steps

- Definition of the Interface in the Instrument Setup for E-mail support.
- Definition of the trigger which exports data to the E-mail program.
- Definition of parameters for E-mail support.

System Requirements 19.2.1

SampleTrack V2.35

ScriptLib V3.3

DB V2.039

E-mail Internal Processes 19.2.2

The following internal processes are performed when using the E-mail notification in SampleTrack. First a database trigger generates a dataset in the table INTERF_TRIG_TAB, which provides a list of samples, for which an E-mail notification needs to be performed. This trigger is activated in the database each time a sample or an experiment is set to the **Finished** status. The SampleTrack Communication Server scans the INTERF_TRIG_TAB table for available datasets. If a dataset is found, the Communication Server runs the predefined script which executes the E-mail notification. The script contains commands, that are integrated with the Communication Server, which prepare data for E-mail distribution. After finishing this process the current dataset is deleted.

E-mail Interface 19.2.3

Automatic E-mail notification is supported by the SampleTrack Communication Server. As the Communication Server only supports instruments, an instrument interface must be defined before automatic E-mail notification can be used. The following steps must be performed in order to define an instrument interface:

Select Environment Setup - Instruments from the tree, and press the New button to define a new instrument.

Assign the name EMAIL to the new instrument (all instruments should have capital letters).

Select the instrument type INTERFACE.

Select the script EMAIL_Export from ScriptLib (ScriptLib V3.3 is required).

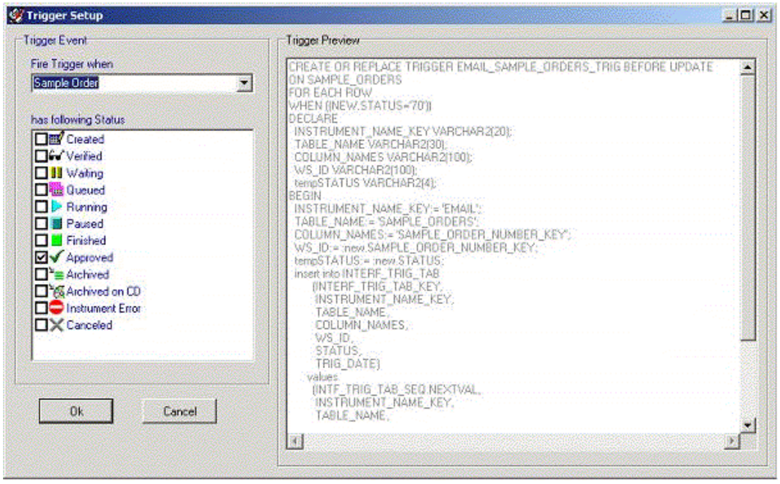
Press the Save button to save all the data to database.

E-mail Trigger Setup 19.2.4

The button **Trigger Setup**, in the Common Settings window, is used to define the event which determines when the E-mail should be sent. Possible events include: experiments, preparations, methods and sample orders. E-mail notification is activated following the completion of one of these events. The event option can be selected from the pull-down box **Fire Trigger When**. After selecting the event option, you must also select one of the checkbox options under **Has Following Status**, which indicates the status of when the trigger should be fired. Standard options for these two parameters are **Status Finished** for the status, and **Sample Order** for the table. On the right side of the Trigger Setup window is the internal database trigger, displayed as SQL text.

To activate the trigger, the checkbox **Use Trigger For Export** must be checked in the Common Settings window.

Figure 19.3. The E-mail Trigger Setup Window



Fire Trigger when: Sample Order

has following Status

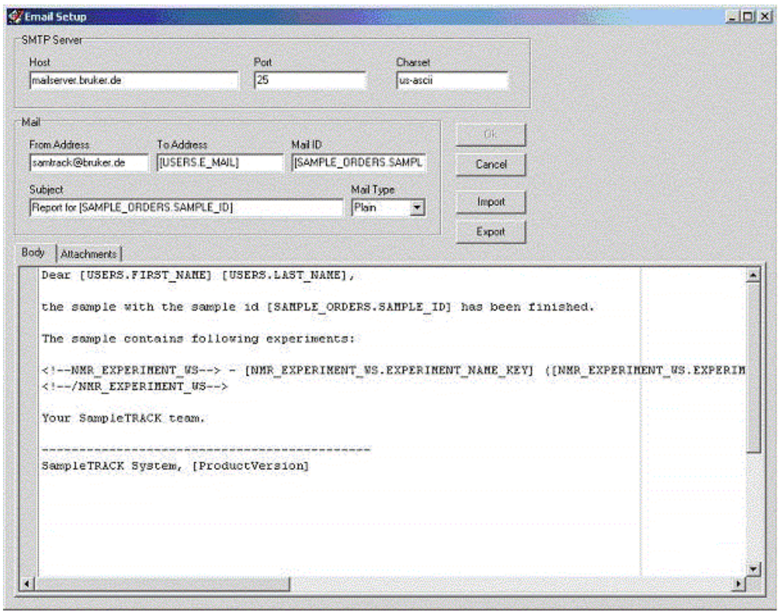
☐ Created
☐ Verified
☐ Waiting
☐ Queued
☐ Running
☐ Paused
☐ Finished
☑ Approved
☐ Archived
☐ Archived on CD
☐ Instrument Error
☐ Canceled

```
CREATE OR REPLACE TRIGGER EMAIL_SAMPLE_ORDERS_TRIG BEFORE UPDATE
ON SAMPLE_ORDERS
FOR EACH ROW
WHEN ((NEW.STATUS='70'))
DECLARE
 INSTRUMENT_NAME_KEY VARCHAR2(20);
 TABLE_NAME VARCHAR2(30);
 COLUMN_NAMES VARCHAR2(100);
 WS_ID VARCHAR2(100);
 tempSTATUS VARCHAR2(4);
BEGIN
 INSTRUMENT_NAME_KEY:= 'EMAIL';
 TABLE_NAME := 'SAMPLE_ORDERS';
 COLUMN_NAMES:= 'SAMPLE_ORDER_NUMBER_KEY';
 WS_ID:= :new.SAMPLE_ORDER_NUMBER_KEY;
 tempSTATUS:= :new.STATUS;
 insert into INTERF_TRIG_TAB
      (INTERF_TRIG_TAB_KEY,
       INSTRUMENT_NAME_KEY,
       TABLE_NAME,
       COLUMN_NAMES,
       WS_ID,
       STATUS,
       TRIG_DATE)
     values
      (INTF_TRIG_TAB_SEQ.NEXTVAL,
       INSTRUMENT_NAME_KEY,
       TABLE_NAME,
```

E-mail Parameters *19.2.5*

To edit the E-mail parameters press the button **E-mail**, which will open an E-mail parameter dialog window.

Figure 19.4. E-mail Parameters



Host: mailserver.bruker.de
Port: 25
Charset: us-ascii

From Address: samtrack@bruker.de
To Address: [USERS.E_MAIL]
Mail ID: [SAMPLE_ORDERS.SAMPL
Subject: Report for [SAMPLE_ORDERS.SAMPLE_ID]
Mail Type: Plain

```
Dear [USERS.FIRST_NAME] [USERS.LAST_NAME],

the sample with the sample id [SAMPLE_ORDERS.SAMPLE_ID] has been finished.

The sample contains following experiments:

<!--NMR_EXPERIMENT_WS--> - [NMR_EXPERIMENT_WS.EXPERIMENT_NAME_KEY] ([NMR_EXPERIMENT_WS.EXPERIM
<!--/NMR_EXPERIMENT_WS-->

Your SampleTRACK team.

---------------------------------------------
SampleTRACK System, [ProductVersion]
```

E-mails can be configured as HTML or plain text format. The following information must be modified:

Field	Value	Description
Host	<your smtp server host>	Host where the E-mails will be sent.
Port	25	Port for SMTP server.
Charset	US-ASCII	Different locales have different character sets. Default is US-ASCII.
User	Samtrack	Name of E-mail sender
Mail ID	SAMPLE_ORDERS.SAMPLE_ID]	Unique identifier, to identify E-mail.
Subject	Sample ‘[SAMPLE_ORDERS.SAMPLE_ID]’ finished	Title for the E-mail.
Attachments	[SAMPLE_ORDERS.DOCU_FILES]	Attachments that should be sent with the E-mail.

The following fields are contained in the mail context: one header, one or more body entries (dependant on the number of experiment datasets) and one footer.

Header

The following experiments in the sample order [SAMPLE_ORDERS.SAMPLE_ID] are finished:

Body

[NMR_EXPERIMENT_WS.EXPERIMENT_NAME_KEY] on
[NMR_EXPERIMENT_WS.INSTRUMENT_NAME_KEY]

Text for bodies. Mail can consist of several entries.

Footer

Please remember to pick up you plots.

Thank you for choosing SampleTrack.

Text for footer information.

Note: Once you have finished the configuration, you must restart the Communication Server in order for the changes to take effect.

E-mail Interface Trigger Table *19.2.6*

Description for INTERF_TRIG_TAB

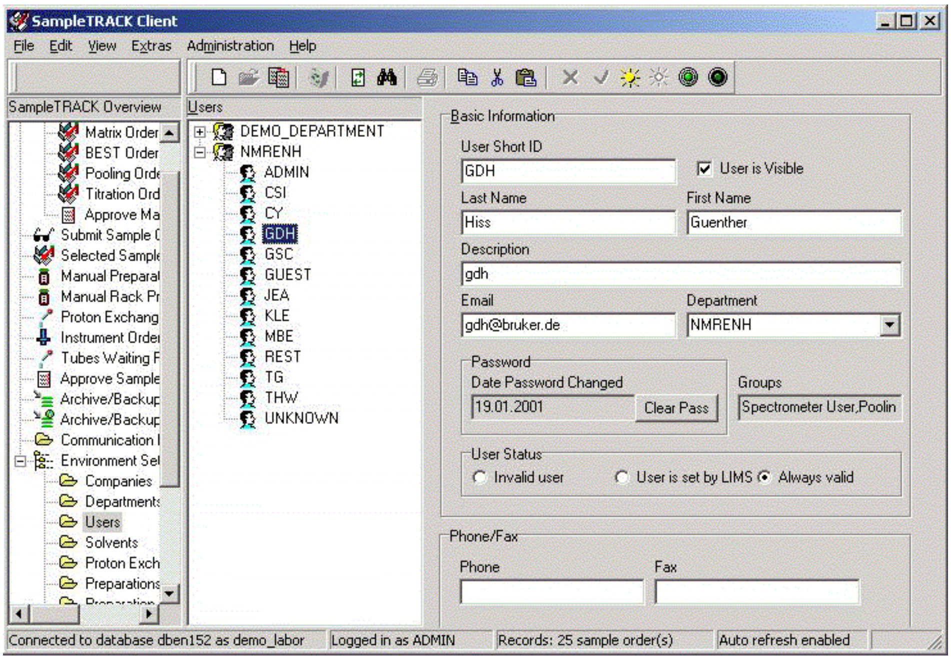
The following fields have been predefined for the INTERF_TRIG_TAB table:

Field Name	**Type**	**Description**
INTERF_TRIG_PK	Number (22)	Unique internal number.
INSTRUMENT_NAME_KEY	Varchar (20)	Interface (instrument) name; dependant on the trigger instrument (will be set for E-mail support instrument: E-mail).
TABLE_NAME	Varchar (30)	The name of the table that has fired the trigger.
COLUMN_NAMES	Varchar (100)	Reference fields that identify the dataset (SAMPLE_ORDER_NUMBER_KEY, METHOD_TYPE_KEY, NMR_PREPARATION_WS_KEY, NMR_EXPERIMENT_WS_KEY).
WS_ID	Varchar (100)	Reference values that identify the dataset (1234,NMR, 1235,1236).
STATUS	Varchar (4)	The status that has fired the trigger.
TRIG_DATE	Date	The date and time when the trigger was fired.

E-mail Address Registering 19.2.7

The E-mail address is registered in the environment user setup

Figure 19.5. E-mail Address in the Environment User Setup



User Short ID: GDH

☑ User is Visible

Last Name: Hiss

First Name: Guenther

Description: gdh

Email: gdh@bruker.de

Department: NMRENH

Date Password Changed: 19.01.2001

Groups: Spectrometer User,Poolin

User Status: ○ Invalid user ○ User is set by LIMS ● Always valid

Connected to database dben152 as demo_labor | Logged in as ADMIN | Records: 25 sample order(s) | Auto refresh enabled

Data Exchange & Directory Structure

20

Introduction to Data Exchange 20.1

SampleTrack™ contains several predefined table structures that are used for the organization and display of key data both internally and in external programs. This chapter provides a description of the individual fields used in these table structures.

There are several fields found in the four base tables used internally by SampleTrack™. Refer to Introduction to SampleTrack Base Tables for details.

There are also several fields that are used by the view VCU_REQUEST_ALL. This view is used when viewing data from an external program such as Crystal Reports™ or Microsoft® Excel®. Refer to the Description of the VCU_REQUEST_ALL Tables for details.

SampleTrack™ bstsdata Directory Structure 20.2

When using the SampleTrack™ software it is essential that the following directory structure is created as described below:

All instrument directories must be located in a directory labeled bstsdata.

For each instrument there must be a separate subdirectory with the specific instrument name. These instrument subdirectories must consist of the necessary in and out directories which are used for file communication.

The **In directory** is where instrument input files are to be located.

Instrument	File Type
LIMS	SampleTrack™ report files for the company LIMS
PREP	Preparation order files from SampleTrack™
SPECT	Spectrometer order files from SampleTrack™

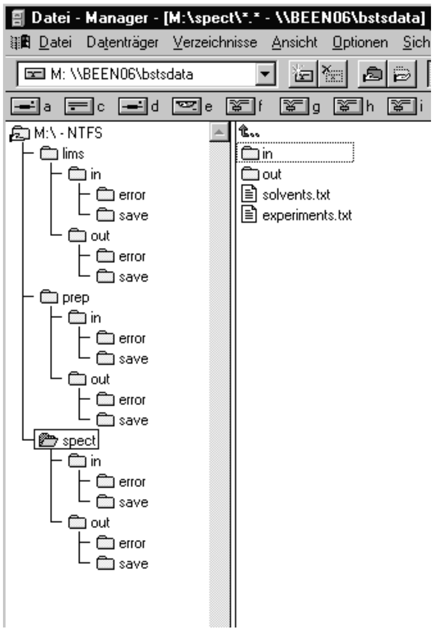
The **Out directory** is where the instrument reports are to be located.

Instrument	File Type
LIMS	LIMS work lists for SampleTrack™ import
PREP	Preparation report files from SampleTrack™
SPECT	Spectrometer report files from SampleTrack™

Each In or Out directory must contain a save and an error sub-directory.

When the files have been accessed successfully by the SampleTrack™ system, or any other instrument, they are moved to the associated save directory.

When the access was unsuccessful (e.g. a syntax error) the files are moved to the error directory.



JCAMP Definition File

21

JCAMP Definition File Introduction 21.1

The communication files serve as the exchange between SampleTrack™ and the served instruments and systems like spectrometers, preparation robots or LIMS.

Each instrument has a separate In and Out directory defined for its information exchange.

In Directory:

Order-File created by SampleTrack

Information:SampleTrack --> Instrument

Out Directory:

Report-File created by Instrument

The **Report File** contains the status or result of a measurement or preparation order.

Several files can be generated for one order.

Information:Instrument --> SampleTrack

The control software for each instrument scans the In directory for current orders, reads the incoming files and reports the results into the out directory. The Out file structure is the same as the incoming file structure completed with the result and order status information.

Workflow Example:

SampleTrack generates an order file for the preparation robot for each preparation .

File name: Sample-ID.[*]p(valid file nomenclature: abc123.p – abc123.10p – acb123.11p – abc123.102p)

After the preparation the preparation robot writes the report file:

File name:Sample-ID.[*]r

SampleTrack generates for each experiment / measurement an order file for the spectrometer.

File name: Tube-ID.10r; Tube-ID.11r

The spectrometer generates for each experiment / measurement 2 report files.

File name: Tube-ID.11s (**Status**-Info 1.Exp); Tube-ID.12s (**Result**-Info 1. Exp.)
Tube-ID.13s (**Status**-Info 2.Exp); Tube-ID.14s (**Result**-Info 2. Exp.)

Communication File with JCAMP Format *21.2*

A communication file includes two parts: Header and variable part.

The header rows are preceded by two hash marks (##). The header information is defined by the universal JCAMP format.

The variable part is preceded by the hash and dollar symbols (##$). Variables preceded by ##$ are user defined and in alphabetcal order.

Header:

##TITLE= Setup File, SampleTrack Software Version x.x

(x.x The current version number)

##JCAMPDX= 5.0

(JACMP Version)

##DATATYPE= Parameter Values

(Data or parameter file)

##ORIGIN= BRUKER BIOSPIN GMBH

(Responsible company name)

##OWNER= Client company, that uses the data

Variable Part:

##$ACAMREQUEST= NOT USED

(Table: NMR_EXPERIMENT_WS . AC_AM_REQUEST)

Special requests for AC or AM instruments.

‘YES’ or empty

Format: string (max. 40 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer.

##$ACCOUNT= NOT USED

(Table: DEPARTMENTS.COST_CENTER)

The client cost center

Format: string (max. 40 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer --> JCAMP data file.

##$ANALYST=

(Table: NMR_EXPERIMENT_WS . USER_NAME_KEY)

Spectrometer operators ID (Not necessarily the logged in user).

Format: string (10 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer --> JCAMP data file.

##$BESTMETHOD=

(Table: SAMPLE_ORDERS . USER_NAME_KEY)

Client user ID

Format: string (10 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer --> JCAMP data file.

##$CLIENTCODE=

(Table: SAMPLE_ORDERS . USER_NAME_KEY)

Client ID

Format: string (10 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer --> JCAMP data file.

##$CLIENTDEPARTMENT=

(Table: USERS . DEPARTMENT_NAME_KEY)

Client department ID

Format: string (max. 40 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer --> JCAMP data file.

##$CLIENTEXPERIMENT= NOT USED

(Table: NMR_EXPERIMENT_WS.CLIENT_EXPERIMENT)

Format: string (max. 40 digits).

--> Realized with parameter ##$EXPERIMENT.

##$CLIENTNAME=

(Table: COMPANIES . COMPANY_NAME)

Company name

Format: string (max. 40 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer--> JCAMP data file.

##$CLIENTSOLVENT= NOT USED

(Table: NMR_PREPARATION_WS.CLIENT_SOLVENT)

Client solvent: H2O,THF,DMSO,D2O,CDCL3,...

Format: string (max. 40 digits).

--> Realized with parameter ##$SOLVENT.

##$COMPOSIT_BASE_EXPNO =

(Table: NMR_EXPERIMENT_WS . COMPOSIT_BASE_EXPNO)

Virtual basis experiment number of a composit experiment. No spectra.

--> Generated by spectrometer.

--> Interpreted by SampleTrack.

When the composit experiment is restarted, this field is transfered to ICON-NMR™:

--> Generated by SampleTrack

--> Interpreted by spectrometer.

##$COMPOSITEXPERIMENT=

(Table: NMR_EXPERIMENT_WS . COMPOSIT_EXPERIMENT)

Composit experiment name as defined in the spectrometer software.

This experiment is not necessarily defined within the SampleTrack experi

ment tables.

Format: string (max. 256 digits)

--> Generated by spectrometer.

--> Interpreted by SampleTrack.

##$COMPOSITMULTIORDERFILES

(Table: BSTS_REGISTRY -- DEFAULT_JCAMP_VALUES - Value)

Switches between the possibility of decomposing a composite experiment within SampleTrack (1) or the spectrometer software (0). When the decomposition takes place in the spectrometer software (0), SampleTrack generates the order with one experiment.

--> Generated by SampleTrack.

--> Interpreted by spectrometer.

##$COMPOSITSEQNUMBER=

(Table: NMR_EXPERIMENT_WS . COMPOSIT_SEQ_NUMBER)

The composite experiment sequence number followed by comma (,) and the number of experiments belonging to the composite experiment.

Format: n,m

--> Generated by spectrometer.

--> Interpreted by SampleTrack.

##$DANGER=   NOT USED

(Table: SAMPLE_ORDERS . DANGER_HINT)

Indicates dangerous attributes of a sample like

toxic, biohazard, radioactive, irritant, flammable, cancer hazard, ...

Format: string (max. 40 digits).

--> Possibly generated by SampleTrack.

##$DATASETNAME= NOT USED

Directory path name of the result file

Format: string (max. 40 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer.

##$DISKUNIT=

(Table: NMR_EXPERIMENT_WS . DISKUNIT)

Target directory (default: /u)

Format: ASCII string (max. 50 digits).

--> Generated by SampleTrack .

--> Interpreted by spectrometer (ICON-NMR™).

##$DISPOSE= NOT USED

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack.

--> Interpreted by AutoPREP.

##$EXPERIMENT_WS_ID=

(Table: NMR_EXPERIMENT_WS . NMR_EXPERIMENT_WS_KEY)

Unique experiment ID

Format: ASCII string.

--> Generated by SampleTrack

--> Interpreted by SampleTrack.

##$EXPERIMENT=

(Table: NMR_EXPERIMENT_WS . EXPERIMENT_NAME_KEY)

Experiment name: 13C,31P,1H,1R,GC-IR,GC-MS,MS,...

Format: ASCII string (max. 256 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer.

##$EXPERIMENTEND= <Stunde : Minute Monat / Tag / Jahr>

(Table: NMR_EXPERIMENT_WS . DATE_END)

Format: ASCII string (max. 40 digits)

--> Generated by Spectrometer.

--> Interpreted by SampleTrack.

##$EXPERIMENTNUMBER=

(Table: NMR_EXPERIMENT_WS . EXPERIMENT_NUMBER)

ExpNo

Part of RESULTDATAPATH.

--> Generated by Spectrometer.

--> Interpreted by SampleTrack.

Restart Experiment:

--> Generated by SampleTrack.

--> Interpreted by spectrometer.

##$EXPERIMENTSTART= <Hour : Minute Month / Day / YEARr>

(Table: NMR_EXPERIMENT_WS . DATE_START)

Format: ASCII string (max. 40 digits).

--> Generated by Spectrometer.

--> Interpreted by SampleTrack.

##$EXPERSTATUS=

(Table: NMR_EXPERIMENT_WS . STATUS)

Order status SampleTrack --> Spectrometer.

Possible entries: NEWPROBE or ADDITIONAL.

(SampleTrack --> Spectrometer).

measurement status Spectrometer --> SampleTrack.

Possible entries: ENDOK, ENDERR, WORKING.

(Spectrometer --> SampleTrack).

The error message can be attached in case of an error (ENDERR), separated by a space.

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack or Spectrometer.

--> Interpreted by SampleTrack or Spectrometer.

#$FILTER=

(Table: NMR_PREPARATION_WS . FILTER)

Indicates the use of a paper filter.

Possible entries: 0, 1.

--> Generated by SampleTrack.

--> Interpreted by AutoPREP.

##$INSTRUMENT=

(Table: NMR_EXPERIMENT_WS . INSTRUMENT_NAME_KEY)

Indicates the analysis instrument for an experiment e.g. DPX300

Format: ASCII string (20 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer.

##$JCAMPRESULTFILE=

field exists for compatibility reasons.

Use **JCAMPRESULTFILE_REAL** instead.

(Table: NMR_EXPERIMENT_WS . JCAMP_RESULT_FILE)

Path and file name of processed data (REAL) in JCAMP format.

(source: [1D: 1r] [2D: still open]).

Format: ASCII string (max. 40 digits).

--> Generated by Spectrometer.

--> Interpreted by SampleTrack.

Example JCAMPRESULTFILE.

##$JCAMPRESULTFILE_RAW=

(Table: NMR_EXPERIMENT_WS . JCAMP_RESULT_FILE)

Path and file name of raw data (FID, SER) in JCAMP format.

(source: [1D: fid] [2D: still open]).

Format: ASCII string (max. 40 digits).

--> Generated by Spectrometer.

--> Interpreted by SampleTrack.

See example JCAMPRESULTFILE.

##$JCAMPRESULTFILE_REAL=

(Table: NMR_EXPERIMENT_WS . JCAMP_RESULT_FILE)

Path and file name of processed data (REAL) in JCAMP format.

(source: [1D: 1r] [2D: still open]).

Format: ASCII string (max. 40 digits).

--> Generated by Spectrometer.

--> Interpreted by SampleTrack.

See example JCAMPRESULTFILE

##$JCAMPRESULTFILE_REAL_IMAG=

(Table: NMR_EXPERIMENT_WS . JCAMP_RESULT_FILE)

Path and file name of processed data (REAL and IMAG) in JCAMP format.

(source: [1D: 1r und 1i] [2D: still open]).

Format: ASCII string (max. 40 digits).

--> Generated by Spectrometer.

--> Interpreted by SampleTrack.

See example JCAMPRESULTFILE

##$JOURNAL=

(Table: METHODS . JOURNAL_NUMBER)

Indicates the labor journal number.

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer.

##$MAXTEMP=

(Table: NMR_PREPARATION_WS . MAX_TEMP)

Maximum sample or solvent temperature.

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack.

--> Interpreted by the preparation robot.

##$MINTEMP=

(Table: NMR_PREPARATION_WS . MIN_TEMP)

Minimum sample or solvent temperature.

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack.

--> Interpreted by the preparation robot.

##$NMRPARAMS=

(Table: NMR_EXPERIMENT_WS . PARAMS)

Experiment parameters seperated by semicolons.

Parameter name and its value are seperated by a blank.

Example:ns 20;sw 10.

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack.

--> Interpreted by the preparation robot.

##$ORDERNUMBER=

(Table: SAMPLE_ORDERS . SAMPLE_ORDER_NUMBER_KEY)

Internal unique order number.

Format: ASCII string (20digits).

--> Generated by SampleTrack.

-->Interpreted by SampleTrack.

##$PHDEMAND= NOT USED

(Table: NMR_PREPARATION_WS .)

Required PH value.

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack .

--> Interpreted by the preparation robot.

##$PREPARATION_WS_ID=

(Table: NMR_PREPARATION_WS . NMR_PREPARATION_WS_KEY)

Unique key of the preparation record.

Format: ASCII string.

--> Generated by SampleTrack.

--> Interpreted by SampleTrack.

##$PREPARATIONDATE= <Hour : Minute Montht / Day / Year>

(Table: NMR_PREPARATION_WS . DATE_END)

End of preparation.

Format: ASCII string (max. 40 digits).

--> Generated by the preparation robot.

--> Interpreted by SampleTrack.

##$PREPARATIONOPERATOR=

(Table:NMR_PEPARATION_WS.USER_NAME_KEY)

(or NMR_PEPARATION_WS.PREPARATION_OPERATOR_NAME)

ID of the chemist doing the preparation.

Format: ASCII string (20 digits).

--> Generated by SampleTrack.

##$PREPSTATUS=

(Table: NMR_PREPARATION_WS . STATUS)

Order status preparation robot --> SampleTrack.

Possible entries: ENDOK, ENDERR, WORKING.

The error message can be attached in case of an error (ENDERR), separated by a space.

Format: ASCII string (max. 40 digits).

--> Generated by the preparation robot.

--> Interpreted by SampleTrack.

##$PROTONEXCHANGE=

(Table: NMR_PREPARATION_WS . PROTON_EX_NAME_KEY)

Indicates the solvent for a proton exchange.

Example: D2O, ...

Used by the spectrometer software by extending.

##$SAMPLETITLE with [##$PROTONEXCHCHANGE]-Exchange for the plot

Format: ASCII string (20 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer.

##$RESULTDATAPATH=

Example RESULTDATAPATH.

(Table: NMR_EXPERIMENT_WS . RESULT_DATA_PATH)

FID path name (raw data) after measurement.

A combination of several spectrometer variables like SPECTROMETER OPERATOR, SAMPLEID and EXPERIMENTNUMBER.

Example: /u/data/guest/nmr/AB000134/10.

SPECTROMETEROPERATOR = guest.

SAMPLEID = AB000134.

EXPERIMENTNUMBER = 10.

Format: ASCII string (max. 40 digits).

--> Generated by Spectrometer.

--> Interpreted by SampleTrack.

##$RETURNDATE=   NOT USED

Format: <Monat/Tag/Jahr> ASCII string (max. 40 digits)

##$ROUT_POS= NOT USED

(NMR_EXPERIMENT_WS.WS_POSITION)

Format: ASCII string (max. 80 digits).

--> Generated by SampleTrack.

--> Interpreted by SampleTrack.

##$SAMPLEAMOUNT=

(NMR_PREPARATION_WS . SAMPLE.AMOUNT)

Sample substance in mg.

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack .

--> Interpreted by the preparation robot.

##$SAMPLECHANGERHOLDER=

(Table: NMR_EXPERIMENT_WS . SAMPLE_CHANGER_HOLDER)

Sample position within the B-ACS carousel.

Format: ASCII string (max. 40 digits).

--> Generated by Spectrometer (when reading the tubeID-Barcode).

or manually entered (MANUPREP) with urgent sample orders.

--> Interpreted by SampleTrack or Spectrometer (URGENT).

##$SAMPLEID=

(Table: SAMPLE_ORDERS.SAMPLE_ID)

Identification of the sample substance.

Format: ASCII string (10 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer.

##$SAMPLENATURE= NOT USED

(Table: SAMPLE_ORDERS.SAMPLE_NATURE)

State of sample aggregation like solid, liquid, semifluid, crystalline.

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack .

##$SAMPLETITLE=

(Table: SAMPLE_ORDERS . SAMPLE_TITLE)

Plot title.

Format: ASCII string (max. 240 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer.

##$SENSITIVE= NOT USED

Sample qualities like light, hygroscopic...

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack.

##$SETUPDATE=   NOT USED

(Table: SAMPLE_ORDERS.DATE_ENTRY)

Order setup or entry date.

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack.

##$SETUP_FILE=

ICON-NMR™ uses this variable temporarily.

It holds the order file name in a report file.

Example: 1234.10r

Format: ASCII string (max. 40 digits).

--> Generated by Spectrometer.

--> Evaluation for debugging only.

##$SPECTROMETEROPERATOR=

(Table: NMR_EXPERIMENT_WS . INSTRUMENT_LOGIN_NAME)

Spectrometer User. If the variable #USER is empty, it fills up the #RESULTDATAPATH with the UserID.

Format: ASCII string (20 digits).

--> Generated by Spectrometer.

--> Interpreted by SampleTrack.

##$SOLVAMOUNT=

(Table: NMR_PREPARATION_WS . SOLVENT_AMOUNT)

Solvent amount in ml.

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack.

--> Interpreted by the preparation robot.

##$SOLVENT=

(Table: NMR_PREPARATION_WS . SOLVENT_NAME_KEY)

Used solvent ID like H2O,THF,DMSO,D2O,CDCL3,...

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack.

--> Interpreted by preparation robot.

--> Interpreted by spectrometer.

##$SOLVMETHOD=

(Table: NMR_PREPARATION_WS .
SOLVENT_MIX_METHOD_NAME_KEY)

Used solvent method like USONIC, HEATER...

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack .

--> Interpreted by the preparation robot.

##$SOLVTEMP=

(Table: NMR_PREPARATION_WS . SOLVENT_MIX_TEMP)

Solvent temperature.

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack .

--> Interpreted by the preparation robot.

##$SOLVTIME=

(Table: NMR_PREPARATION_WS . SOLVENT_MIX_TIME)

Solvent duration.

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack .

--> Interpreted by the preparation robot.

##$TUBEHANDLING= NOT USED

Tube handling like 4mm,top melting, coding, vacuum, ...

Format: ASCII string (max. 40 digits).

--> Generated by SampleTrack.

##$TUBEID=

(Table: METHODS . TUBE_ID)

Temporarily sample identifikation during the measurement:

It is the ID on the barcode collar tube. The tube ID is entered when the preparation takes place, either manually, by hand scanner or with the B-BCE instrument.

Format: ASCII string (max. 40 digits).

--> Generated by the preparation robot.

--> Interpreted by SampleTrack und Spectrometer.

##$ URGENT =

(Table: SAMPLE_ORDER . URGENT_SAMPLE_ORDER)

Urgent orders are measured before others.

Valid entries: 1 or 0

--> Generated by SampleTrack

--> Interpreted by spectrometer

##$ USER =

(Table: NMR_EXPERIMENT_WS .USER_NAME_KEY)

User ID - known in the spectrometer software and ICON-NMR™

Part of RESULTDATAPATH.

Format: ASCII string (20 digits).

--> Generated by SampleTrack.

--> Interpreted by spectrometer.

Script Library

22

Introducing Scripts for Automation 22.1

The package **stscript.bpl** (Module: dmScript.pas) is used for SampleTrack Client, Easy Dialog and Communication Server.

It includes routines for automation to store custom specific configurations.

Available commands are most of the commands used in Delphi 6.0

The following sections describe the common variables and functions.

Common Variables and Functions 22.2

Variables with Instrument Type: Interface 22.2.1

vFileName File name for Import or Export (read/write).

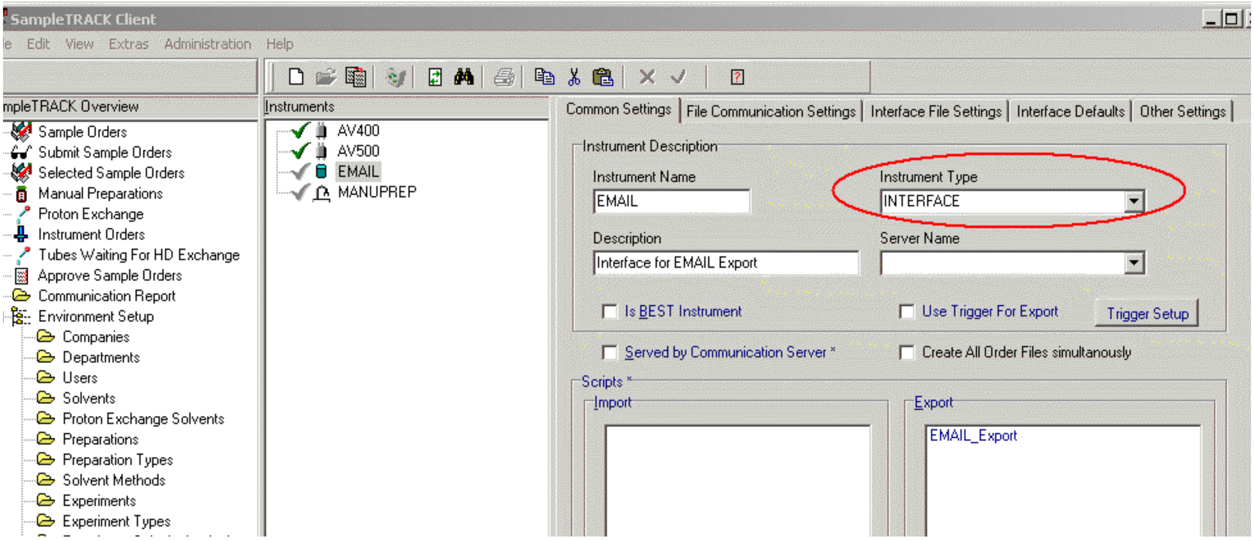
vMethod Method Name, default is the content from vDefMethodName (usually ‘NMR’).

vScriptName (RO)Name of the running scripts.

vInstrumentName (RO)Name of the current instrument.

vTransactionError (RO)Boolean-Variable within the program (StComSrv) that indicates a transaction error.

*Figure 22.1. Instrument Type **Interface***



Instrument Name: EMAIL

Instrument Type: INTERFACE

Description: Interface for EMAIL Export

Server Name:

☐ Is BEST Instrument

☐ Use Trigger For Export

☐ Served by Communication Server *

☐ Create All Order Files simultanously

Export: EMAIL_Export

Columns on Tab 'Interface File Settings' *22.2.2*

vClientIdCol (RO)

vExperimentCol (RO)

vHdExchangeCol (RO)

vSampleIdCol (RO)

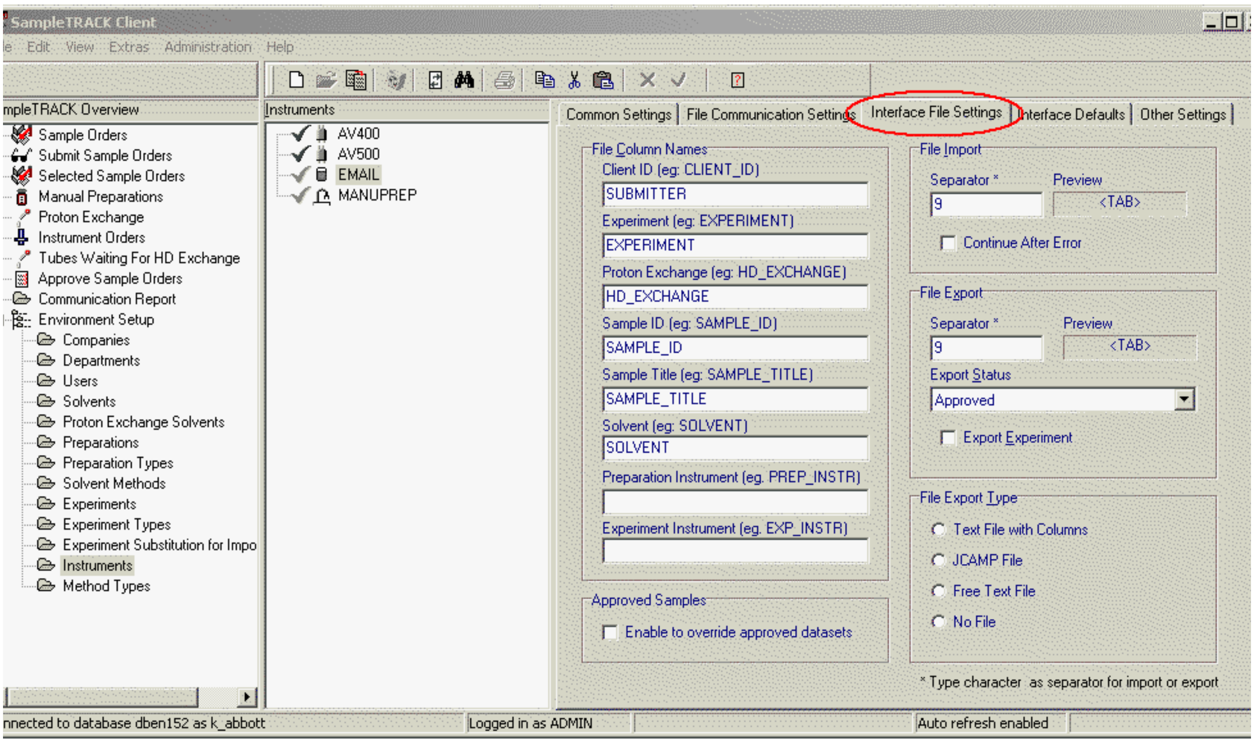
vSampleTitleCol (RO)

vSolventCol (RO)

vPrepInstrCol (RO)

vExpInstrCol (RO)

Figure 22.2. Interface File Settings



File Column Names

Client ID (eg: CLIENT_ID): SUBMITTER

Experiment (eg: EXPERIMENT): EXPERIMENT

Proton Exchange (eg: HD_EXCHANGE): HD_EXCHANGE

Sample ID (eg: SAMPLE_ID): SAMPLE_ID

Sample Title (eg: SAMPLE_TITLE): SAMPLE_TITLE

Solvent (eg: SOLVENT): SOLVENT

Preparation Instrument (eg. PREP_INSTR):

Experiment Instrument (eg. EXP_INSTR):

Approved Samples

☐ Enable to override approved datasets

File Import

Separator *: 9 Preview: <TAB>

☐ Continue After Error

File Export

Separator *: 9 Preview: <TAB>

Export Status: Approved

☐ Export Experiment

File Export Type

○ Text File with Columns

○ JCAMP File

○ Free Text File

○ No File

* Type character as separator for import or export

nnected to database dben152 as k_abbott | Logged in as ADMIN | Auto refresh enabled

fClientId	Field content of vClientIdCol (global variable, editable)
fExperiment	Field content of vExperimentCol (global variable, editable)
fHdExchange	Field content of vHdExchangeCol (global variable, editable)
fSampleId	Field content of vSampleIdCol (global variable, editable)
fSampleTitle	Field content of vSampleTitleCol (global variable, editable)
fSolvent	Field content of vSolventCol (global variable, editable)
fPrepInstr	Field content of vPrepinstrCol (global variable, editable)
fExpInstr	Field content of vExpInstrCol (global variable, editable)

vDefSoStartStatus (RO)Start status Sample Order for the current instrument vDefMNmrStartStatus (RO)Start status methods (NMR), for the current instrument

vDefNpwStartStatus (RO)Start status Nmr_Preparation_Ws for the current instrument

vDefNewStartStatus (RO)Start status Nmr_Experiment_Ws for the current instrument

vDefMMsStartStatus (RO)Start status methods (MS) for the current instrument

vDefMpwStartStatus (RO)Start status Nmr_Preparation_Ws for the current instrument

vDefMewStartStatus (RO)Start status Nmr_Experiment_Ws for the current instrument

vDefCompanyName (RO)Company Name

vDefDepartmentName (RO)Department Name

vDefNmrExpInstrName (RO)Default NMR Spectrometer Instrument

vDefNmrPrepInstrName (RO)Default NMR Preparations Instrument

vDefMethodName (RO)Default Method

Common Terms for Script Processing *22.3*

SO ‘SAMPLE_ORDERS’

M ‘METHODS’

NPW ‘NMR_PREPARATION_WS’

NEW ‘NMR_EXPERIMENT_WS’

UNCHECKED‘0’

CHECKED‘1’

When a table is opened multiple times, the record can be identified using an alias name + ’_’ + a consecutive number, rather than using table names.

Example: (always beginning with ’1’)

SAMPLE_ORDERS_1

SAMPLE_ORDERS_2

NMR_EXPERIMENT_WS_1

NMR_EXPERIMENT_WS_2

etc.

Functions for Script Processing *22.3.1*

Procedure Self.Abort#

Stops the current processing.

Transaction and post_transaction_script will be performed.

Procedure Self.Exit#

Ends the current script. The script(s) that follow will be carried out.

Procedure Self.SetGlobVar#(VariableName, Value: String).

Allows the definition of global variables valid within a list of scripts.

Function Self.GetGlobVar#(VariableName: String): String

Delivers the value of a variable that was set previously.

If not defined, the value returned is an empty String.

Function Self.ConvertToFieldName#(Text: String): String

Converts a text into data base field name format and returns it as a String.

Function ShellExecute#(Operation, FileName, Parameter, Directory: String.

ShowMode: Integer): Boolean.

Executes a command.

Operation defines the action to be executed, e.g. **Open**. Filename is the name of the commando file or the file to be opened. **Parameter** are the parameters passed to **FileName**. **Directory** is the working directory. **Showmode** indicates the size of the new window.

1	= Minimized
2	= Maximized
No entry	= Normal

Functions for File Import/Export 22.3.2

Function Self.GetFileFieldCount#: Integer.

Returns the number of fields from the standard I/O file.

Function Self.GetFileFieldName# (Index: Integer): String.

Returns the column name from the I/O file.

Function Self.GetFileValue#(ColumnName: String): String.

Returns the column content from the I/O file.

Function Self.SetFileValue#(ColumnName, Value: String): Boolean.

Writes a value into the column of the I/O file.

Function Self.OpenJCAMPFileTable#(FileName, AliasTableName: String): Boolean.

Opens an optional JCAMP file. This file can be used additionally to the standard I/O file. Fields are handled as table fields.

Function Self.OpenTextFileTable#(FileName, AliasTableName: String.

HasHeadline: Boolean; Separator: Char): Boolean.

Opens a text file as a table.

This file can be used additionally to the standard I/O file.

Fields are handled as table fields.

Function Self.SetTextColumns#(Table, FieldNames: String): Boolean.

Defines, which columns to be used.

Column separator is „;".

Function Self.ReadTextLine#(Table: String; var Line: String): Boolean.

Adds a line to the file.

Function Self.WriteTextLine#(Table, Line: String): Boolean.

Writes a line to the file

String Manipulation

Function Self.Extract#(var OrgString: String; Sep: String): String.

Extracts the next column field from a field list with

column separator **Sep**

Functions for Tables 22.4

Function Self.GetSequenceNumber(SequenceName: String): String.

Returns the next sequence number

Function Self.ExecStoredProc(aProc: String): String.

Returns the return value of a stored procedure

Function Self.OpenTable(Table, LookupColumnNames, LookupValues, OrderBy: String.

ReadOnly: Boolean): Boolean.

Opens a table for repeated read or write.

The first record found with the where clause is the current record.

(Conditional on LookupColumnNames, LookupValues)

Return value: Record exists (True/False)

Function Self.CloseTable(Table: String): Boolean.

Closes the table

Function Self.GetTableState(Table: String): Integer.

Returns the table status:

0=EOF; 1=browse; 2=insert; 3=edit

Function Self.GetTableCountOf(Table: String): Integer.

Returns the number of tables in the list **aTable**

Function Self.ReadFromTable(Table, ColumnName: String.

var ResultString :String): Boolean.

Returns a value of an opened table. Additionally field contents from the table EXT_FIELDS can be returned.

Those fields must be predefined in the DB Registry.

Return value: Record exists (True/False)

Function Self.WriteToTable(Table, ColumnName, Value: String): Boolean.

Writes into an opened table.

Additional fields can be written into table EXT_FIELDS as defined in the DB Registry.

Function Self.SaveTable(Table: String): Boolean.

Saves the current Record into the Database

Function Self.InsertToTable(Table: String): Boolean.

Saves the current Record into the Database

Function Self.Locate(Table, LookupColumnNames, LookupValues,

OrderBy: String): Boolean)

Jumps to the first record in a table with a hit on the where clause.

(Conditional on LookupColumnNames, LookupValues)

Function Self.CopyFields(SourceTable, DestinationTable: String): Boolean.

Copies the content of all fields with the same column field from source table to destination table.

Destination table columns containing values will not be overwritten.

Function Self.DeleteRecord(Table: String; CloseTable: Boolean): Boolean.

Deletes the current record and closes the table when CloseTable is TRUE.

Function Self.DeleteFromTable(Table, LookupColumnNames,

LookupValues: String): Boolean.

Deletes one or more records.

Function Self.SetMethodsStatus(aSampleOrderNumberKey, aStatus: String): Boolean.

Sets the status for all worksteps and methods.

Returns TRUE on success.

The Tube ID is released when the status >= 70 und status<>90.

Function Self.SetWSStatus(aWSTable, aWSKey, aStatus: String): Boolean.

Sets the status of the workstep.

Worksteps are preparations and experiments. The superior status must be set by the function RecreateStatus.

Function Self.RecreateStatus(aTable, aKey: String): Boolean.

Checkes the method and sample order status. Conditionally modifies the status when required.

Releases the tube ID when the status >= 70 and status <> 90.

Sample Order: self.Recreate(SO, '1234')

Methods: self.Recreate(M, '1234;NMR')

Function Self.GotoFirstRecord(aTable: String): Boolean.

Sets the cursor to the first record in the table aTable. The table must be opened before. Returns FALSE when the table was not found.

Function Self.GotoLastRecord(aTable: String): Boolean.

Sets the cursor to the last record in the table aTable. The table must be opened before. Returns FALSE when the table was not found.

Function Self.GotoNextRecord(aTable: String): Boolean.

Sets the cursor to the next record in the table aTable. The table must be opened before. Returns FALSE when the table was not found.

Function Self.GotoPrevRecord(aTable: String): Boolean.

Sets the cursor to the previous record in the table aTable. The table must be opened before. Returns FALSE when the table was not found.

Function Self. GotoRecordNumber (aTable: String; aLine): Boolean.

Sets the cursor to the specified record in the table aTable. The table must be opened before. Returns FALSE when the table was not found.

Function Self.BOF(aTable: String): Boolean.

Returns TRUE when when the first record is hit by the function GotoPrevDataset or is hit by the function GotoFirstDataset.

Returns TRUE when the file set is empty or the table was not found.

Function Self.EOF(aTable: String): Boolean.

Returns TRUE when when the last record is hit by the function GotoNextDataset or is hit by the function GotoLastDataset.

Returns TRUE when the file set is empty or the table was not found.

Function Self.RecordCount(aTable: String): Integer.

Returns the number of rows of a file set

Function Self.CancelTable(aTable: String): Boolean.

Cancels the changes

Function Self.RenameTable(aOldTable, aNewTable: String): Boolean.

Renames the table for further processing

Lookup Functions Database 22.5

Function Self.LookupTableValue(Table, LookupColumnNames, LookupValues, ResultColumnName: String; var ResultString: String): Boolean.

Looks up a value in a table and closes the table

Returns: Record found (True/False)

Function Self.GetInstrumentDefaultValue(Instrument, Title: String. var ResultString: String): Boolean.

Returns the title within the section I_<Instrument>

Returns: Record found (True/False)

Function Self.GetDefaultValue(Title: String; var ResultString: String): Boolean.

Returns the title content within the section I_<aktuelles Instrument>

Returns: Record found (True/False)

Function Self.GetGlobalDefaultValue(Method, Title: String; var ResultString: String): Boolean.

Returns the title content from the section

GLOBALS or GLOBALS_<Method>.

In case the String **Method** is empty, the section GLOBALS is inquired in the following.

Returns: Record found (True/False)

Function Self.ConvertToUNC(aInstrument, aPath: String): String.

Converts an instrument path to UNC

Function Self.GetDBTime(Dummy: Integer): String.

Returns the current database date and time

Format: '10:00 03/22/1999'

Function Self.GetDBRegistryEntry(aUser, aSection, aTitle, aDefault: String. aField: Integer): String.

Returns a value from the DB Registry

aField indicates the kind of information: 0=Value, 1=Desc, 2=Memo1, 3=Memo2

Function Self.GetAliasName(aTableName, aFieldName: String): String.

Returns the column alias name

Field / Value Evaluation 22.6

Function Self.IsValidString(aText: String; aUseUpperLetters, aUseLowerLetters, aUseFigures: Boolean; aCustomChars: String): Boolean;

Checks for a valid String

Function Self.IsValidFloat(aText, aRangeString: String.
aRangeIncrement: String): Boolean.

Checks for a valid floating point number

Function Self.IsValidInteger(aText, aRangeString: String;
aRangeIncrement: String): Boolean.

Checks for a valid number

Procedure Self.CheckValidFieldString(aTableName, aFieldName: String;
aUseUpperLetters, aUseLowerLetters, aUseFigures: Boolean;
aCustomChars: String).

Checks for a valid field String

Procedure Self.CheckValidFieldFloat(aTableName, aFieldName: String;
aRangeString: String; aRangeIncrement: String).

Checks for a valid field floating point number.

Procedure Self.CheckValidFieldInteger(aTableName, aFieldName: String;
aRangeString: String; aRangeIncrement: String).

Checks for a valid field number.

Show Messages 22.7

Procedure Self.ShowMessage(MessageString: String).

Shows a message.

Procedure Self.ShowError(ErrorString: String).

Shows an error message. The script processing is aborted for the current loop.

(Internal Exception).

Procedure Self.ShowDatasetFields(aTable: String).

Displays the current fields and their content.

Function: Send Emails 22.8

Function Self.SetMailParams(aHost, aPort, aUserID, aCharSet: String): Boolean.

Configures E-mail with common parameters.

Function Self.SetMailID(aSampleID: String): Boolean.

Places an identifier to send the E-mail automatically when the identifier changes.

Function Self.SetMailFrom(aFromAddress, aFromName, aReplyTo: String): Boolean.

Defines the E-mail sender

Function Self.SetMailTo(aToAddress, aToCarbonCopy, aToBlindCarbonCopy: String): Boolean.

Defines the E-mail receiver.

Function Self.SetMailSubject(aSubject: String): Boolean.

Defines the E-mail title.

Function Self.SetMailHeader(aHeader: String): Boolean.

Defines the E-mail header.

Function Self.SetMailFooter(aFooter: String): Boolean.

Defines the E-mail footer.

Function Self.AddMailBody(aBody: String): Boolean.

Defines an E-mail body block.

Function Self.ClearMailBody: Boolean.

Deletes an E-mail body block.

Function Self.AddMailAttachment(aAttachment: String): Boolean.

Adds an attachment to the E-mail.

Function Self.ClearMailAttachments: Boolean.

Deletes the E-mail attachment list.

Function Self.SendMail: Boolean.

Sends the E-mail.

Function Self.ClearMessage: Boolean.

Deletes the complete E-mail content.

Special Functions 22.9

Function Self.GetExperimentID(SO, NEW: String):String.

Returns a new experiment ID for an experiment.

The experiment type must be known, otherwise the sample ID is returned. The format is defined in the DB Registry:

Globals\Experiment_ID_Mask.

Function Self.CheckForDelayedExperiment(NEW: String):Boolean.

Checks if the experiment (current record) must be set to the status DELAYED. In that case the status and the start date is modified. The function returns TRUE.

Function Self.DoExperimentSubstitution(NEW, Experiment: String):Boolean.

Performs an experiment substitution if an appropriate value in the table Exp_Substitions exists.

This Function may generate several experiments as defined in Exp_Substitions.

Returns TRUE when a substitution takes place.

Function Self.DoHDExchange(NPW, HDInstrument, HDSolvent: String):Boolean.

Adds a preparation with HD Exchange (if not already existing).

Returns TRUE if already existing.

Function Self.CheckForCompositExperiments:Boolean.

Checks the internal dataset list for a composite experiment. If not, sub experiments are added.

Returns TRUE if COMPOSITMULTIORDERFILES=1

Function Self.ClearInvalidOrderFiles(aInstrument: String):Boolean.

Delete invalid order files for the given instrument. When the parameter aInstrument is empty all the order files for all the instruments of type **EXP** are checked for invalid orders.

Function Self.GetNewMethod(aSOKey, aMethodType: String): String.

Generates a new method of type aMethodType for the sample order key aSOKey.

Example: Self.GetNewMethod(1234, ’NMR’)=’NMR-2’).

Function Self.CheckTubeIDStatus(aMethodTable: String): Boolean.

Checks, if the Tube ID is already used in the method table and inserts it where applicable.

Function: Archiving *22.10*

Function Self.GetCurrentDir(aDir: String; aLevel: Integer = 0): String.

Returns the last directory name of a directory path name.

aLevel > 0 indicates the number of parent directories up to the root.

Example: C:\a\b\c\d\e

getcurrentDir(Dir,0) returns e

getcurrentDir(Dir,1) returns d\e

Function Self.GetParentDir(aDir: String; aLevel: Integer = -1): String.

Returns the complete path of the parent directory.

Example: Example: C:\a\b\c\d\e

GetParentDir(dir,1) returns C:\a\b\c\d

GetParentDir(dir,2) returns C:\a\b\c

Function Self.ArchiveData(aTable, aFieldName, aDestPath, aFileMask: String;

aDescend: Boolean): Boolean.

Archives all files in aFieldName. aFieldName can be a path or a list of file names. aDestPath indicates the destination path. aFileMask indicates the filter for the files to be moved. aDescend indicates, if underlying directories must be archived.

Caution: All the data is deleted in the source directories!

Function Self.CopyData(aTable, aFieldName, aDestPath, aFileMask: String;

aDescend: Boolean): Boolean.

Copies all files in aFieldName. aFieldName can be a path or a list of file names. aDestPath indicates the destination path. aFileMask indicates the filter for the files to be copied. aDescend indicates, if underlying directories must be copied. Copy Data can be used as backup routine.

Function Self.DeleteDataFiles(aTable, aFieldName, aFileMask: String;

aDescend: Boolean): Boolean.

Deletes all files in aFieldName. aFieldName can be a path or a list of file names. aFileMask indicates the filter for the files to be deleted. aDescend indicates, if underlying directories must be deleted.

Caution: Data are deleted!

Function Self.DeleteDataDirs(aTable, aFieldName, aFileMask: String.

aDescend: Boolean; aParentDir: Integer = 0): Boolean.

Deletes all directories when empty. aFileMask indicates the filter for directories to be deleted. aDescend indicates, if underlying directories must be deleted. aParentDir indicates if parent directories should be deleted. aParentDir is the first parent directory.

Caution: Data are deleted!

Function Self.ExecuteArchivingForSO(SOKey, Config: String): Boolean.

Archives SampleOrder with the key SOKey with archiving Method Config.

Caution: This function works only within Import or Export Scripts.

Obsolete Functions *22.11*

Function Self.DeleteDataset(Table: String): Boolean.

Deletes the current record and closes the table.

Replaced by: Self.DeleteRecord verwenden.

Function Self.GotoFirstDataset(aTable: String): Boolean.

Sets the cursor to the first record in table aTable.

The table must be opened before. Returns FALSE if the table is not found.

Replaced by: Self.GotoFirstRecord

Function Self.GotoLastDataset(aTable: String): Boolean.

Sets the cursor to the first record in table aTable.

The table must be opened before. Returns FALSE if the table is not found.

Replaced by: Self.GotoLastRecord

Function Self.GotoNextDataset(aTable: String): Boolean.

Sets the cursor to next record in table aTable.

The table must be opened before. Returns FALSE if the table is not found.

Replaced by: Self.GotoNextRecord

Function Self.GotoPrevDataset(aTable: String): Boolean.

Sets the cursor to the previous record in table aTable.

The table must be opened before. Returns FALSE if the table is not found.

Replaced by: Self.GotoPrevRecord

Function Self.WriteFileHeader(Header: String): Boolean.

Writes the file title.

Use Self.OpenTextFileTable and Self.WriteTextLine for Exports except for JCAMP and Table Files.

Function Self.WriteFileLine(Line: String): Boolean.

Adds a line at EOF.

Use Self.OpenTextFileTable and Self.WriteTextLine for Exports except for JCAMP and Table Files.

Alphabetical List of Function and Procedures *22.12*

Abort

AddMailAttachment

AddMailBody

ArchiveData

BOF

CancelTable

CheckForCompositExperiments

CheckForDelayedExperiment

CheckTubeIDStatus

CheckValidFieldFloat

CheckValidFieldInteger

ClearInvalidOrderFiles
ClearMailAttachments
ClearMailBody

ClearMessage
CloseTable
ConvertToFieldName
ConvertToUNC
CopyData
CopyFields
DeleteDataDirs
DeleteDataFiles
DeleteFromTable
DeleteRecord
DoExperimentSubstitution
DoHDExchange
EOF
ExecStoredProc
ExecuteArchivingForSO

Exit
Extract
GetAliasName
GetCurrentDir
GetDBRegistryEntry
GetDBTime
GetDefaultValue
GetExperimentID
GetFileFieldCount
GetFileFieldName
GetFileValue
GetGlobalDefaultValue
GetGlobVar
GetInstrumentDefaultValue
GetNewMethod

GetParentDir

GetSequenceNumber
GetTableCountOf
GetTableState
GotoFirstRecord
GotoLastRecord
GotoNextRecord
GotoPrevRecord
GotoRecordNumber
InsertToTable
IsValidFloat
IsValidInteger
Locate
LookupTableValue
OpenJCAMPFileTable

OpenTable
OpenTextFileTable
ReadFromTable
ReadTextLine
RecordCount
RecreateStatus
RenameTable
SaveTable
SendMail
SetFileValue
SetGlobVar
SetMailFooter
SetMailFrom
SetMailHeader
SetMailID
SetMailParams

SetMailSubject
SetMailTo
SetMethodsStatus
SetTextColumns
SetWSStatus

ShellExecute

ShowDatasetFields

ShowError

ShowMessage

WriteTextLine

WriteToTable

System Requirements

23

General Hint

23.1

For server, PC and spectrometer software requirements see also the BRUKER SampleTrack™ homepage for Server and Client PC requirements: ***http://www.bruker-biospin.de/NMR/automat/samtrac/samtrac5.html***

Server Requirements

23.2

At least one server is required exclusively for SampleTrack™ based on the following minimum requirements:

Pentium IV, 2 GHz (or faster), 1 GB RAM or better.

60 GB harddisk or larger. As an option an additional harddisk for mirroring. This does not include storage for spectra data.

100/1000 Mbit/s Ethernet connection.

A Windows® 2000 compatible graphics adapter with minimum 1024x768 pixel resolution.

A 17" (or larger) monitor with at least 1024x768 pixel resolution and 75 Hz vertical frequency.

A Windows® 2000 compatible mouse and keyboard.

Microsoft Windows® 2000 / 2003 Server.

ORACLE® Standard Edition 8.1.7 or higher (can be delivered by BRUKER).

Client PC Operation System Requirements 23.3

SampleTrack™ can be installed on existing spectrometer PC's or other compatible systems based on the requirements below:

Pentium IV, 1GB RAM or better.

2 GB free space on harddisk (minimum)

100/1000 Mbit/s Ethernet connection.

A Windows® 2000 compatible graphics adapter with minimum 1024x768 pixel resolution.

A 17" (or larger) monitor with at least 1024x768 pixel resolution and 75 Hz vertical frequency.

A Windows® 2000 compatible mouse and keyboard.

Microsoft Windows® 2000 / 2002 Professional.

ORACLE® Client 8.1.7 or higher (can be delivered by BRUKER).

Spectrometer Software Requirements 23.4

- XWIN-NMR™ 3.1 patch level 11 or higher or TOPSPIN® 1.2 or higher
- ICON-NMR™ 3.1 or higher

Directory Sharing with UNIX Instrument Computers 23.5

In order for data to be exchanged between the instruments in your laboratory and the SampleTrack™ data management system, several defined directories have to be shared. This definition may be handled by various NFS software products or using the SAMBA daemon on your UNIX computer. For installation and support please contact your network administrator.

Oracle® 9 Server and Client Installation

24

ORACLE® 9*i* Database Server Installation 24.1

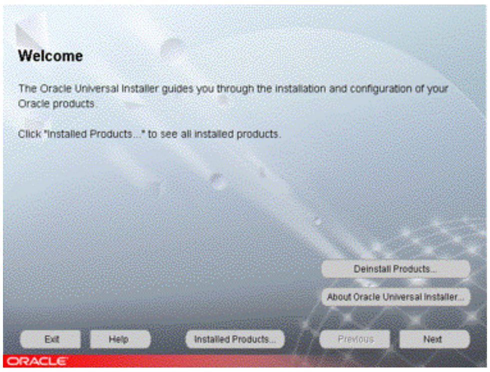
Refer to your Oracle® documentation and provider information for the database installation. The following section may help to prevent common errors that may occur during installation.

For the Oracle® 9i client installation see "ORACLE® 9i Client Installation" on page 186.

The following installation screenshots are dedicated for the database server PC.

Insert the Oracle® CD into CDROM drive - the following Welcome dialog will appear

Figure 24.1. The Oracle® *Welcome Window*



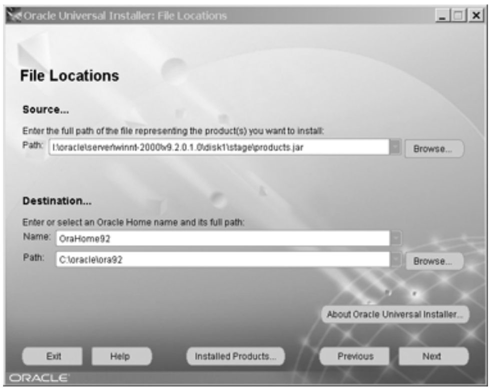
Welcome

The Oracle Universal Installer guides you through the installation and configuration of your Oracle products.

Click "Installed Products..." to see all installed products.

Accept the name OraHome92 and the path C\oracle\ora92

Figure 24.2. The Oracle® *File Locations Window*



Oracle Universal Installer: File Locations

File Locations

Source...

Enter the full path of the file representing the product(s) you want to install:

Path: I:\oracle\server\winnt-2000\v9.2.0.1.0\disk1\stage\products.jar

Destination...

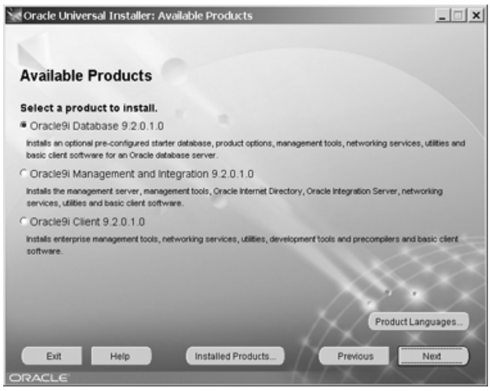
Enter or select an Oracle Home name and its full path:

Name: OraHome92

Path: C:\oracle\ora92

Choose Oracle® 9i database

Figure 24.3. The Oracle® *Available Products Window*



Oracle Universal Installer: Available Products

Available Products

Select a product to install.

● Oracle9i Database 9.2.0.1.0

Installs an optional pre-configured starter database, product options, management tools, networking services, utilities and basic client software for an Oracle database server.

○ Oracle9i Management and Integration 9.2.0.1.0

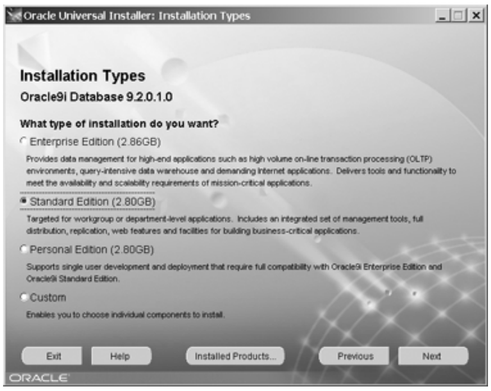
Installs the management server, management tools, Oracle Internet Directory, Oracle Integration Server, networking services, utilities and basic client software.

○ Oracle9i Client 9.2.0.1.0

Installs enterprise management tools, networking services, utilities, development tools and precompilers and basic client software.

Select Standard Edition

Figure 24.4. The Oracle® *Installation Type Window*



Oracle Universal Installer: Installation Types

Installation Types

Oracle9i Database 9.2.0.1.0

What type of installation do you want?

○ Enterprise Edition (2.86GB)

Provides data management for high-end applications such as high volume on-line transaction processing (OLTP) environments, query-intensive data warehouse and demanding Internet applications. Delivers tools and functionality to meet the availability and scalability requirements of mission-critical applications.

● Standard Edition (2.80GB)

Targeted for workgroup or department-level applications. Includes an integrated set of management tools, full distribution, replication, web features and facilities for building business-critical applications.

○ Personal Edition (2.80GB)

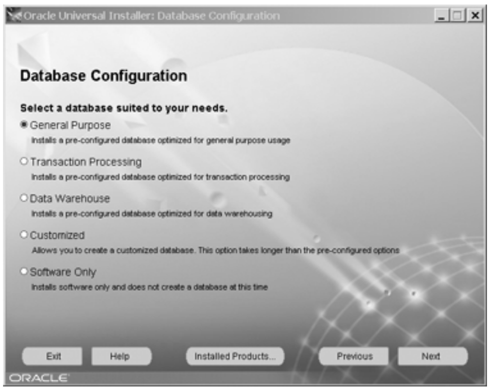
Supports single user development and deployment that require full compatibility with Oracle9i Enterprise Edition and Oracle9i Standard Edition.

○ Custom

Enables you to choose individual components to install.

Select General Purpose

Figure 24.5. The Oracle® *Database Configuration Window*



Database Configuration

Select a database suited to your needs.

● General Purpose
Installs a pre-configured database optimized for general purpose usage

○ Transaction Processing
Installs a pre-configured database optimized for transaction processing

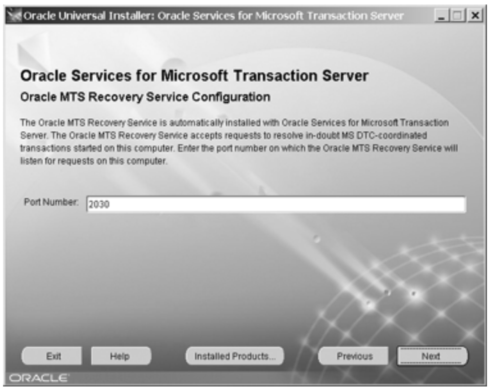
○ Data Warehouse
Installs a pre-configured database optimized for data warehousing

○ Customized
Allows you to create a customized database. This option takes longer than the pre-configured options

○ Software Only
Installs software only and does not create a database at this time

Select standard port number 2030

Figure 24.6. Microsoft® Transaction Server Window


Oracle Universal Installer: Oracle Services for Microsoft Transaction Server
Exit
Help
Installed Products...
Previous
Next
ORACLE

Oracle Services for Microsoft Transaction Server

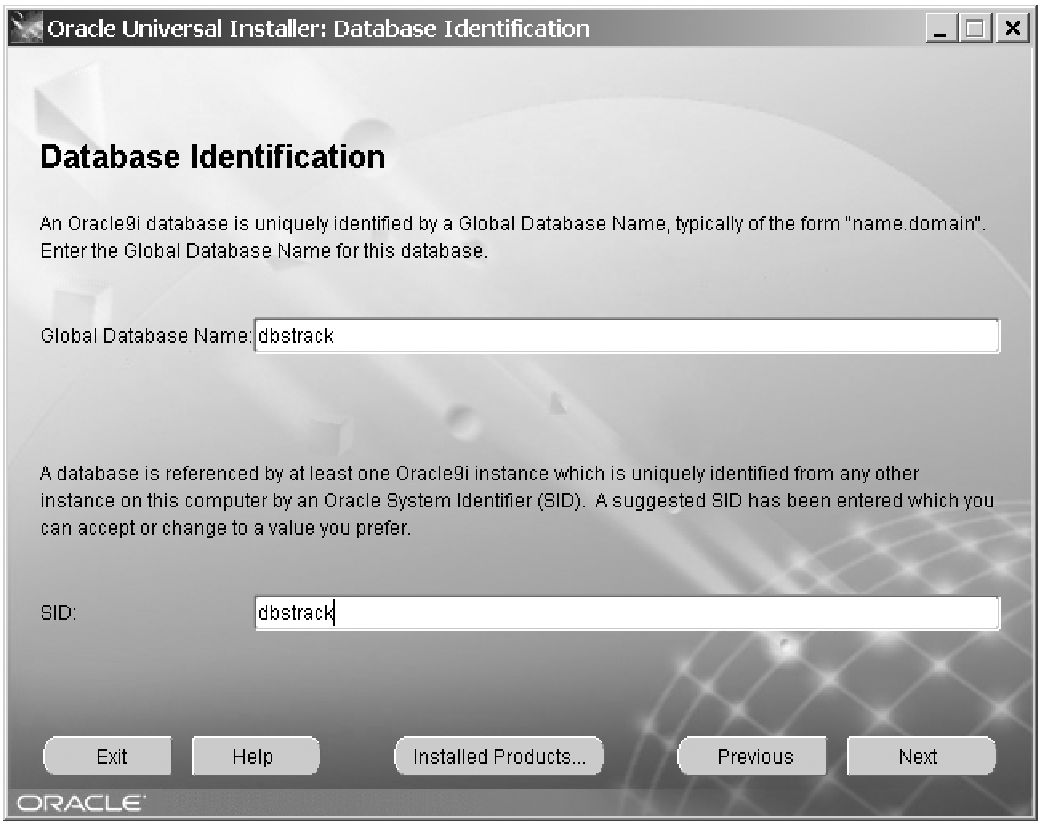
Oracle MTS Recovery Service Configuration

The Oracle MTS Recovery Service is automatically installed with Oracle Services for Microsoft Transaction Server. The Oracle MTS Recovery Service accepts requests to resolve in-doubt MS DTC-coordinated transactions started on this computer. Enter the port number on which the Oracle MTS Recovery Service will listen for requests on this computer.

Port Number: 2030

Select Gobal Database Name dbstrack and SID dbstrack

Figure 24.7. The Oracle® *Database Identification Window*



Database Identification

An Oracle9i database is uniquely identified by a Global Database Name, typically of the form "name.domain". Enter the Global Database Name for this database.

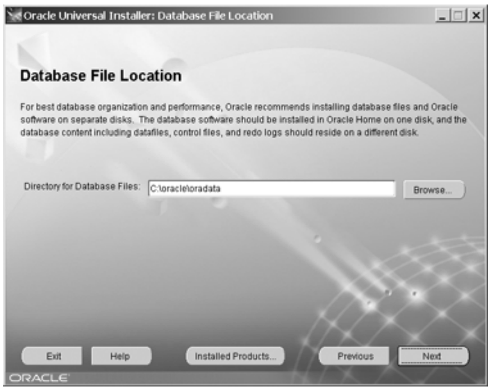
Global Database Name: dbstrack

A database is referenced by at least one Oracle9i instance which is uniquely identified from any other instance on this computer by an Oracle System Identifier (SID). A suggested SID has been entered which you can accept or change to a value you prefer.

SID: dbstrack

Select database file directory C:\oracle\oradata

Figure 24.8. The Oracle® *Database File Location Window*



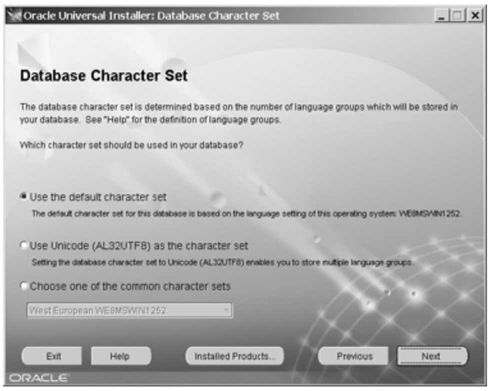
Database File Location

For best database organization and performance, Oracle recommends installing database files and Oracle software on separate disks. The database software should be installed in Oracle Home on one disk, and the database content including datafiles, control files, and redo logs should reside on a different disk.

Directory for Database Files: C:\oracle\oradata

Use the default character set

Figure 24.9. The Oracle® *Database Character Set Window*



Oracle Universal Installer: Database Character Set

Database Character Set

The database character set is determined based on the number of language groups which will be stored in your database. See "Help" for the definition of language groups.

Which character set should be used in your database?

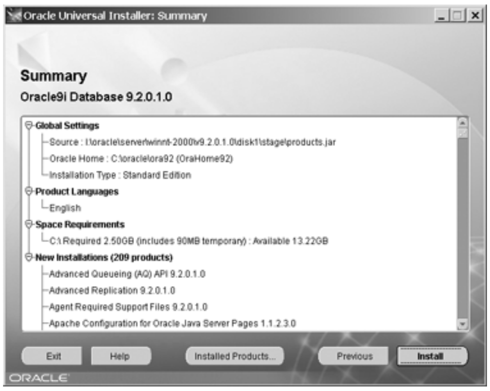
● Use the default character set
The default character set for this database is based on the language setting of this operating system: WE8MSWIN1252.

○ Use Unicode (AL32UTF8) as the character set
Setting the database character set to Unicode (AL32UTF8) enables you to store multiple language groups.

○ Choose one of the common character sets
West European WE8MSWIN1252

Before the installation a summary of the selected items is shown

Figure 24.10.The Oracle® *Summary Window*



Oracle Universal Installer: Summary

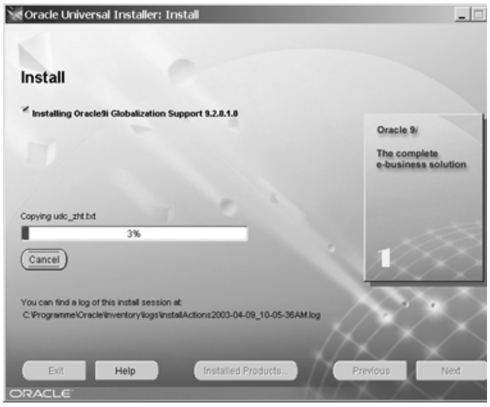
Summary

Oracle9i Database 9.2.0.1.0

- **Global Settings**
  - Source : I:\oracle\server\winnt-2000\v9.2.0.1.0\disk1\stage\products.jar
  - Oracle Home : C:\oracle\ora92 (OraHome92)
  - Installation Type : Standard Edition
- **Product Languages**
  - English
- **Space Requirements**
  - C:\ Required 2.50GB (includes 90MB temporary) : Available 13.22GB
- **New Installations (209 products)**
  - Advanced Queueing (AQ) API 9.2.0.1.0
  - Advanced Replication 9.2.0.1.0
  - Agent Required Support Files 9.2.0.1.0
  - Apache Configuration for Oracle Java Server Pages 1.1.2.3.0

Installation is running

Figure 24.11.The Oracle® *Installation Status Window*



Oracle Universal Installer: Install

Install

Installing Oracle9i Globalization Support 9.2.0.1.0

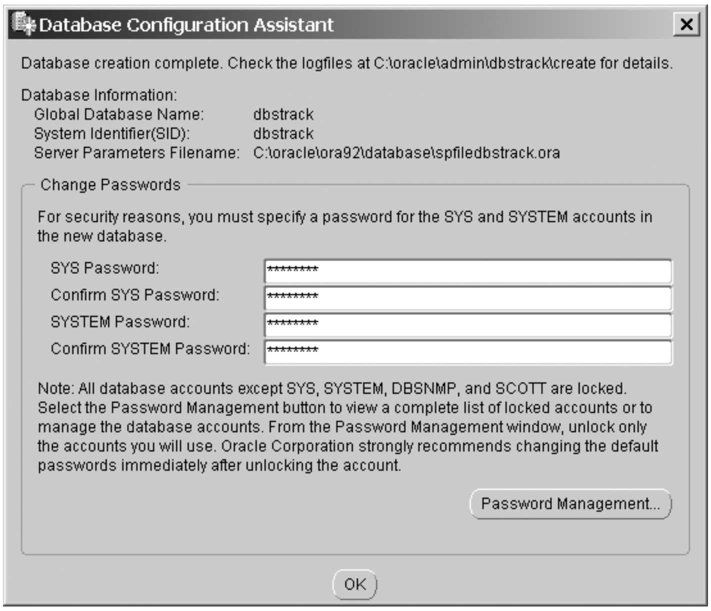
Copying udc_zht.txt

3%

You can find a log of this install session at:
C:\Programme\Oracle\Inventory\logs\installActions2003-04-09_10-05-36AM.log

The configuration assistant lets you modify the sys and system passwords (recommended)

Figure 24.12.The Oracle® *Database Configuration Assistant .*



Database Configuration Assistant

Database creation complete. Check the logfiles at C:\oracle\admin\dbstrack\create for details.

Database Information:
Global Database Name: dbstrack
System Identifier(SID): dbstrack
Server Parameters Filename: C:\oracle\ora92\database\spfiledbstrack.ora

Change Passwords

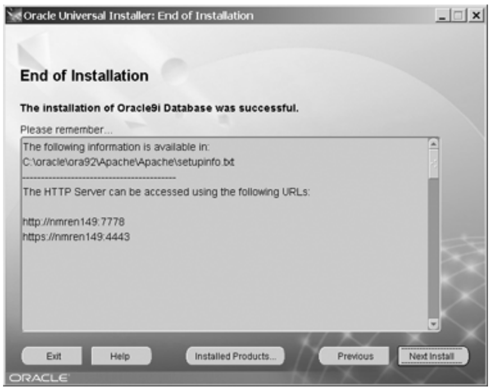
For security reasons, you must specify a password for the SYS and SYSTEM accounts in the new database.

SYS Password: *********
Confirm SYS Password: *********
SYSTEM Password: *********
Confirm SYSTEM Password: *********

Note: All database accounts except SYS, SYSTEM, DBSNMP, and SCOTT are locked. Select the Password Management button to view a complete list of locked accounts or to manage the database accounts. From the Password Management window, unlock only the accounts you will use. Oracle Corporation strongly recommends changing the default passwords immediately after unlocking the account.

Database installation has finished

Figure 24.13.The Oracle® *End of Installation Window*



Oracle Universal Installer: End of Installation

End of Installation

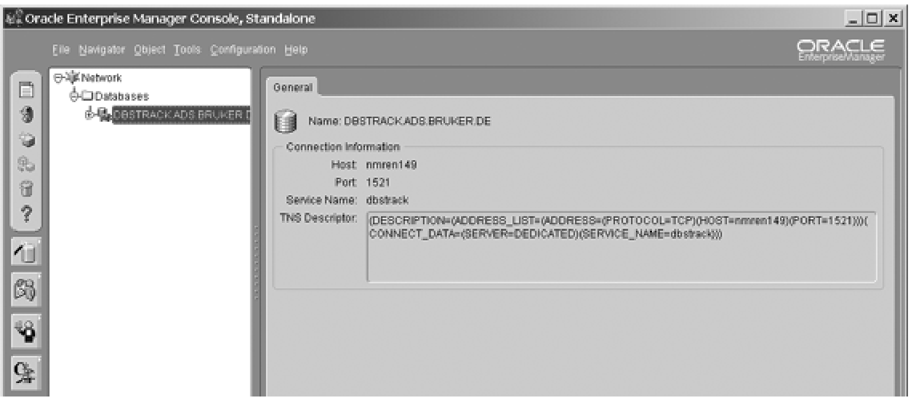
The installation of Oracle9i Database was successful.

Please remember...

```
The following information is available in:
C:\oracle\ora92\Apache\Apache\setupinfo.txt
-----------------------------------------
The HTTP Server can be accessed using the following URLs:

http://nmren149:7778
https://nmren149:4443
```

Find the SampleTrack database within the Enterprise Manager Console

Figure 24.14.Enterprise Manager Console, Standalone Window


Oracle Enterprise Manager Console, Standalone
File Navigator Object Tools Configuration Help
ORACLE
EnterpriseManager
Network
Databases
DBSTRACK.ADS.BRUKER.D
General

Name: DBSTRACK.ADS.BRUKER.DE

Connection Information

Host: nmren149

Port: 1521

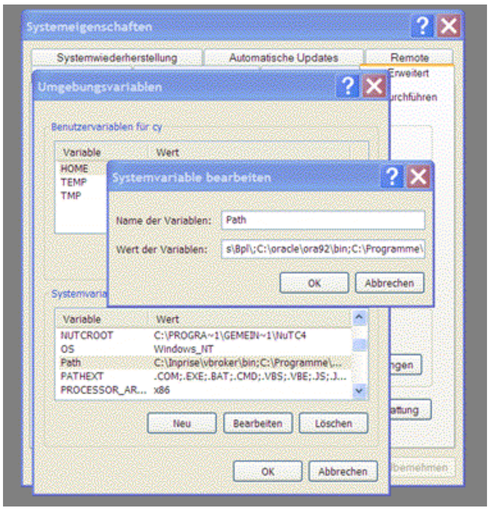
Service Name: dbstrack

TNS Descriptor: (DESCRIPTION=(ADDRESS_LIST=(ADDRESS=(PROTOCOL=TCP)(HOST=nmren149)(PORT=1521)))(CONNECT_DATA=(SERVER=DEDICATED)(SERVICE_NAME=dbstrack)))

The Path in the Environment System 24.1.1

The path “C:\oracle\ora92\bin” must be in the environment system variable, see advanced system properties

Figure 24.15.The Path in the Environment System



Systemvariable bearbeiten

Name der Variablen: Path

Wert der Variablen: s\Bpl\;C:\oracle\ora92\bin;C:\Programme\

Variable	Wert
HOME	
TEMP	
TMP	

Variable	Wert
NUTCROOT	C:\PROGRA~1\GEMEIN~1\NuTC4
OS	Windows_NT
Path	C:\Inprise\vbroker\bin;C:\Programme\...
PATHEXT	.COM;.EXE;.BAT;.CMD;.VBS;.VBE;.JS;.J...
PROCESSOR_AR...	x86

ORACLE® 9i Client Installation *24.2*

Installing Oracle® 9i client on a Windows® PC

Refer to your Oracle® documentation and provider information for the database installation. The following section may help to prevent common errors that may occur during installation.

Version 8 and SampleTrack installation:

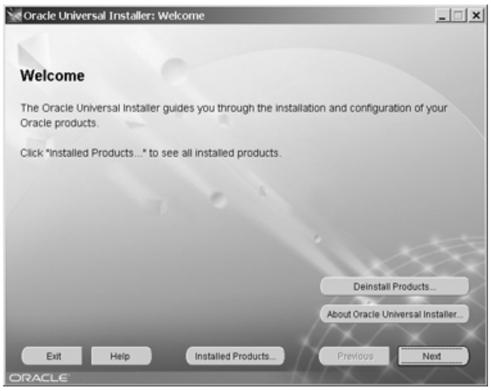
For the installation of Oracle® 8 client installation see the file *Getting Started.pdf* .

The following installation screenshots are dedicated for each PC, where the Oracle® 9i client together with SampleTrack client is needed.

(For the installation of SampleTrack client installation see the file *Getting Started.pdf* .

Insert the Oracle® CD into CDROM drive - the following Welcome dialog will appear

Figure 24.16.The Oracle® *Welcome Window*



Oracle Universal Installer: Welcome

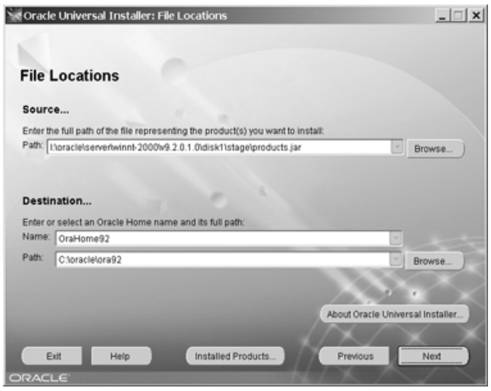
Welcome

The Oracle Universal Installer guides you through the installation and configuration of your Oracle products.

Click "Installed Products..." to see all installed products.

Accept the name OraHome92 and the path C\oracle\ora92

Figure 24.17.The Oracle® *File Locations Window*



Oracle Universal Installer: File Locations

File Locations

Source...

Enter the full path of the file representing the product(s) you want to install:

Path: I:\oracle\server\winnt-2000\v9.2.0.1.0\disk1\stage\products.jar

Destination...

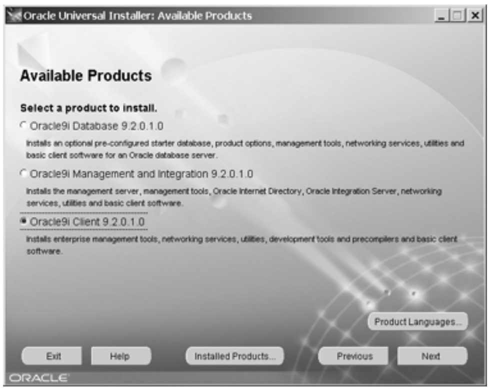
Enter or select an Oracle Home name and its full path:

Name: OraHome92

Path: C:\oracle\ora92

Select the Oracle® client installation

Figure 24.18.The Oracle® *Available Products Window*



Oracle Universal Installer: Available Products

Available Products

Select a product to install.

○ Oracle9i Database 9.2.0.1.0

Installs an optional pre-configured starter database, product options, management tools, networking services, utilities and basic client software for an Oracle database server.

○ Oracle9i Management and Integration 9.2.0.1.0

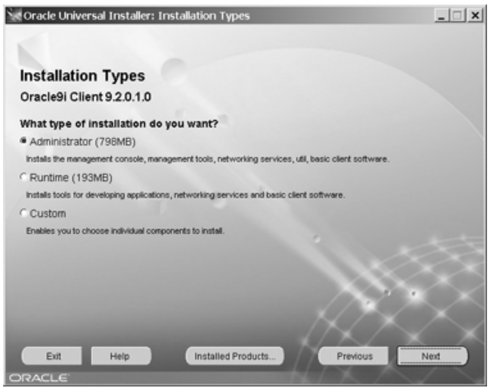
Installs the management server, management tools, Oracle Internet Directory, Oracle Integration Server, networking services, utilities and basic client software.

● Oracle9i Client 9.2.0.1.0

Installs enterprise management tools, networking services, utilities, development tools and precompilers and basic client software.

Select the installation type Administrator

Figure 24.19.The Oracle® *Installation Type Window*



Oracle Universal Installer: Installation Types

Installation Types

Oracle9i Client 9.2.0.1.0

What type of installation do you want?

● Administrator (798MB)

Installs the management console, management tools, networking services, util, basic client software.

○ Runtime (193MB)

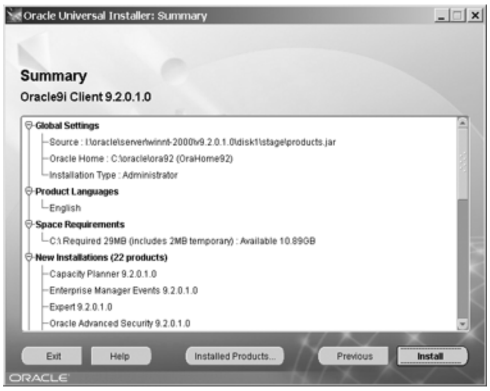
Installs tools for developing applications, networking services and basic client software.

○ Custom

Enables you to choose individual components to install.

Before the installation a summary of the selected items is shown

Figure 24.20.The Oracle® *Summary Window*



Oracle Universal Installer: Summary

Summary

Oracle9i Client 9.2.0.1.0

- **Global Settings**
  - Source : I:\oracle\server\winnt-2000\v9.2.0.1.0\disk1\stage\products.jar
  - Oracle Home : C:\oracle\ora92 (OraHome92)
  - Installation Type : Administrator
- **Product Languages**
  - English
- **Space Requirements**
  - C:\ Required 29MB (includes 2MB temporary) : Available 10.89GB
- **New Installations (22 products)**
  - Capacity Planner 9.2.0.1.0
  - Enterprise Manager Events 9.2.0.1.0
  - Expert 9.2.0.1.0
  - Oracle Advanced Security 9.2.0.1.0

Oracle® 8 Server and Client Installation

25

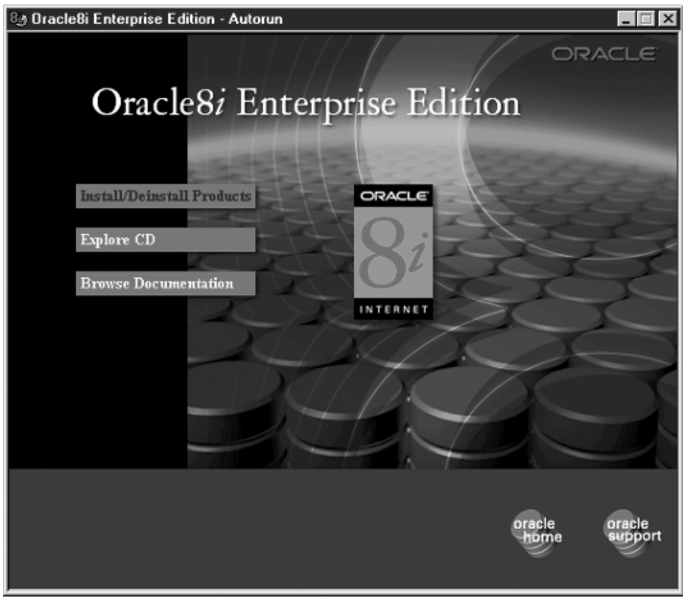
Oracle® 8.1.7. Database Server on a Windows PC 25.1

Refer to your Oracle® documentation and provider information for the database installation. The following section may help to prevent common errors that may occur during installation.

Installation Method 25.2

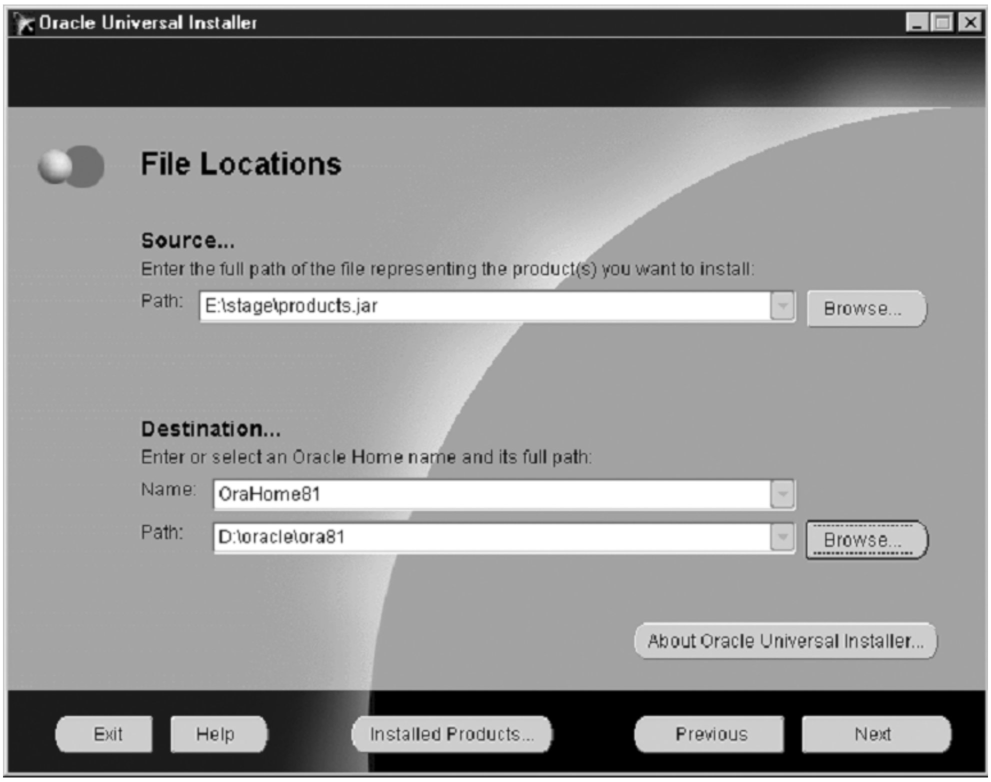
Insert the Oracle® CD into CDROM drive - the following dialog will appear

Figure 25.1. The Oracle® Installation Window:


Oracle8i Enterprise Edition - Autorun
ORACLE
Oracle8*i* Enterprise Edition
Install/Deinstall Products
Explore CD
Browse Documentation
ORACLE
8*i*
INTERNET
oracle home
oracle support

Choose: Install Products

Figure 25.2. The File Locations Window



Oracle Universal Installer

File Locations

Source...

Enter the full path of the file representing the product(s) you want to install:

Path: E:\stage\products.jar

Destination...

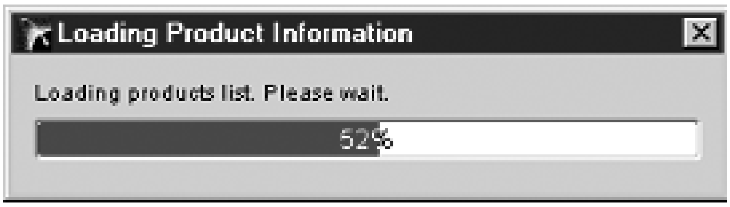
Enter or select an Oracle Home name and its full path:

Name: OraHome81

Path: D:\oracle\ora81

Press: Next

Figure 25.3. The Loading Product Information Window



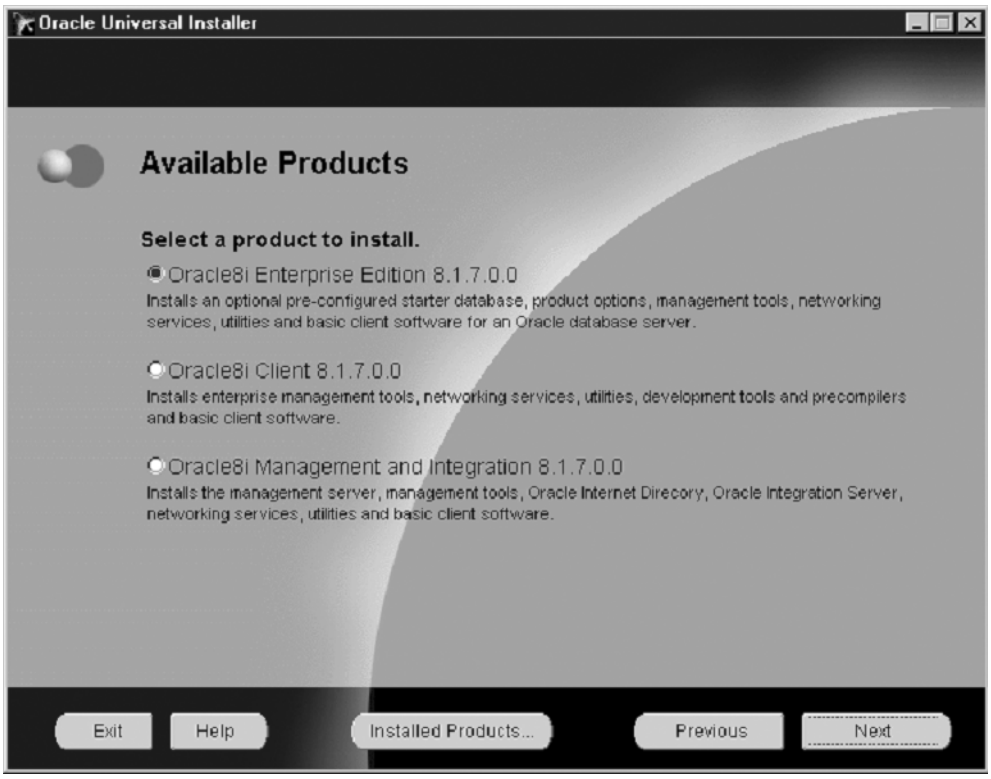
Loading Product Information

Loading products list. Please wait.

52%

Wait...

Figure 25.4. Available Products Window



Available Products

Select a product to install.

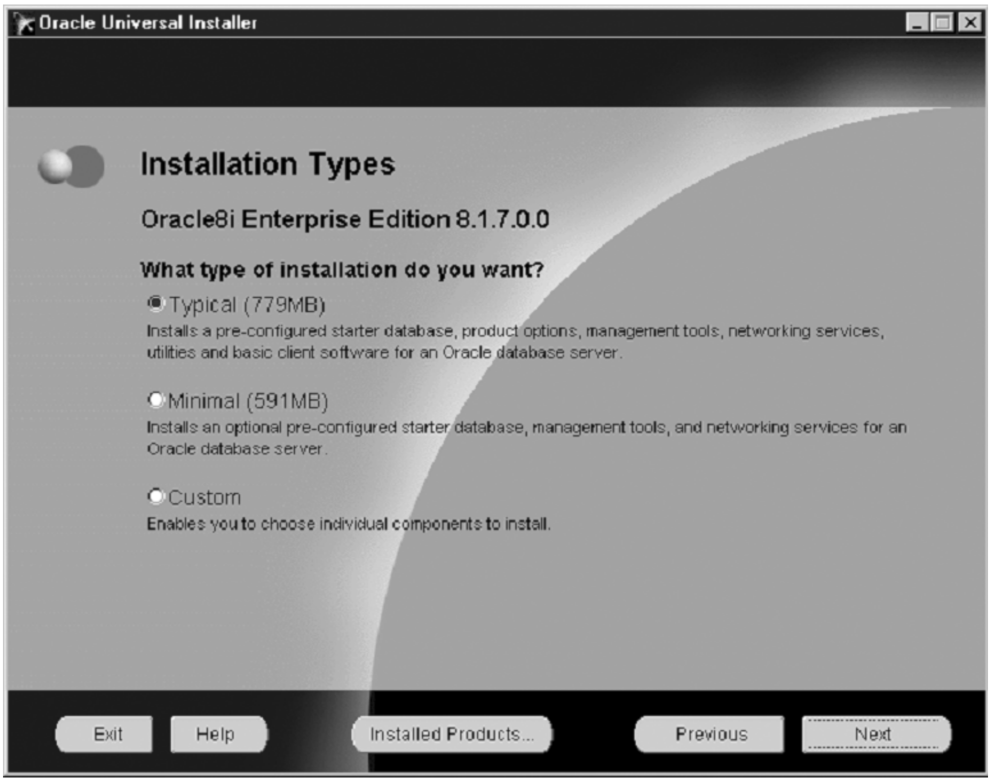
● Oracle8i Enterprise Edition 8.1.7.0.0
Installs an optional pre-configured starter database, product options, management tools, networking services, utilities and basic client software for an Oracle database server.

○ Oracle8i Client 8.1.7.0.0
Installs enterprise management tools, networking services, utilities, development tools and precompilers and basic client software.

○ Oracle8i Management and Integration 8.1.7.0.0
Installs the management server, management tools, Oracle Internet Direcory, Oracle Integration Server, networking services, utilities and basic client software.

Select: Oracle® Enterprise Edition, then press Next

Figure 25.5. Installation Types Window



Installation Types

Oracle8i Enterprise Edition 8.1.7.0.0

What type of installation do you want?

● Typical (779MB)
Installs a pre-configured starter database, product options, management tools, networking services, utilities and basic client software for an Oracle database server.

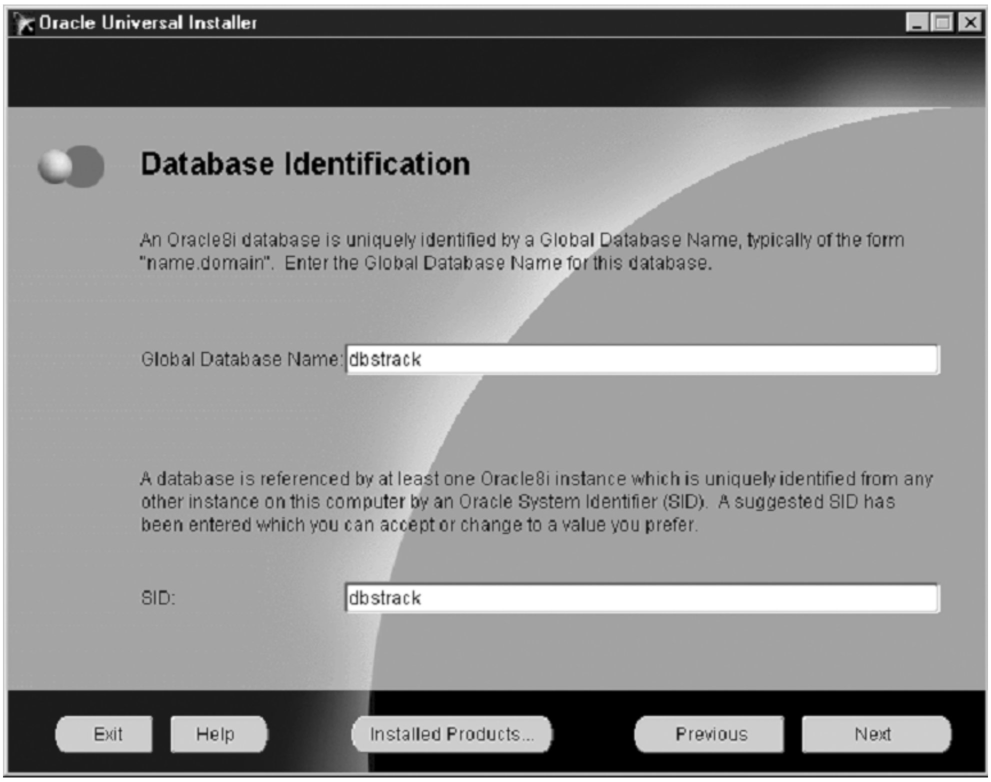
○ Minimal (591MB)
Installs an optional pre-configured starter database, management tools, and networking services for an Oracle database server.

○ Custom
Enables you to choose individual components to install.

Choose: Typical

Press: Next

Figure 25.6. Database Identification Window



Database Identification

An Oracle8i database is uniquely identified by a Global Database Name, typically of the form "name.domain". Enter the Global Database Name for this database.

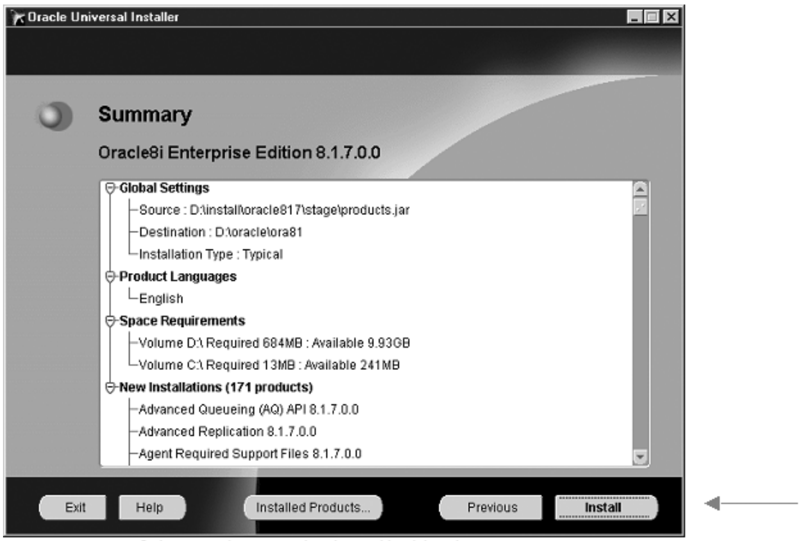
Global Database Name: dbstrack

A database is referenced by at least one Oracle8i instance which is uniquely identified from any other instance on this computer by an Oracle System Identifier (SID). A suggested SID has been entered which you can accept or change to a value you prefer.

SID: dbstrack

For Global Database Name and Instance Name enter: dbstrack

Figure 25.7. Summary Window



Summary

Oracle8i Enterprise Edition 8.1.7.0.0

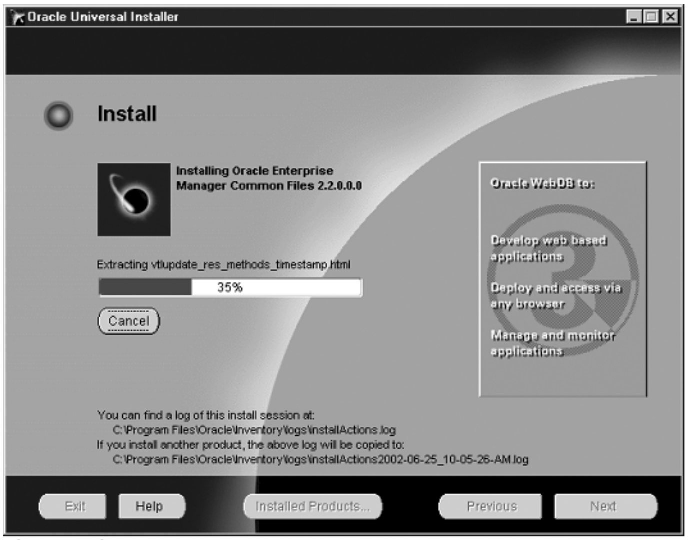
- Global Settings
  - Source : D:\install\oracle817\stage\products.jar
  - Destination : D:\oracle\ora81
  - Installation Type : Typical
- Product Languages
  - English
- Space Requirements
  - Volume D:\ Required 684MB : Available 9.93GB
  - Volume C:\ Required 13MB : Available 241MB
- New Installations (171 products)
  - Advanced Queueing (AQ) API 8.1.7.0.0
  - Advanced Replication 8.1.7.0.0
  - Agent Required Support Files 8.1.7.0.0

A summary of the products to be installed is shown.

A summary of the products to be installed is displayed.

Press Install to continue.

Figure 25.8. Install Progress Window


Oracle Universal Installer
Install
Oracle WebDB to:
Develop web based applications
Deploy and access via any browser
Manage and monitor applications
35%
Cancel
Exit
Help
Installed Products...
Previous
Next

Installing Oracle Enterprise Manager Common Files 2.2.0.0.0

Extracting vtlupdate_res_methods_timestamp.html

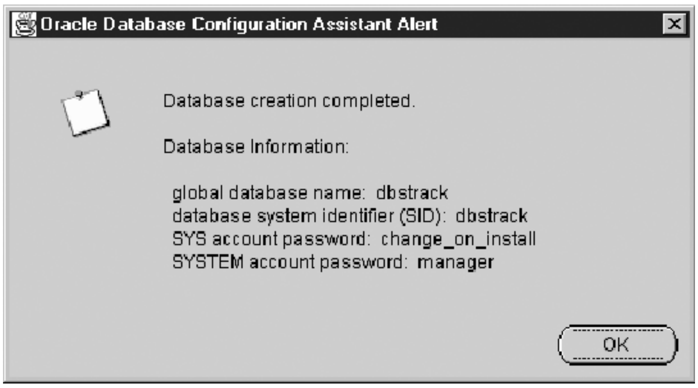
```
You can find a log of this install session at:
    C:\Program Files\Oracle\Inventory\logs\installActions.log
If you install another product, the above log will be copied to:
    C:\Program Files\Oracle\Inventory\logs\installActions2002-06-25_10-05-26-AM.log
```

please wait ...

Wait...

Database creation completed will appear.

Figure 25.9. Oracle® Database Configuration Assistant Alert Window



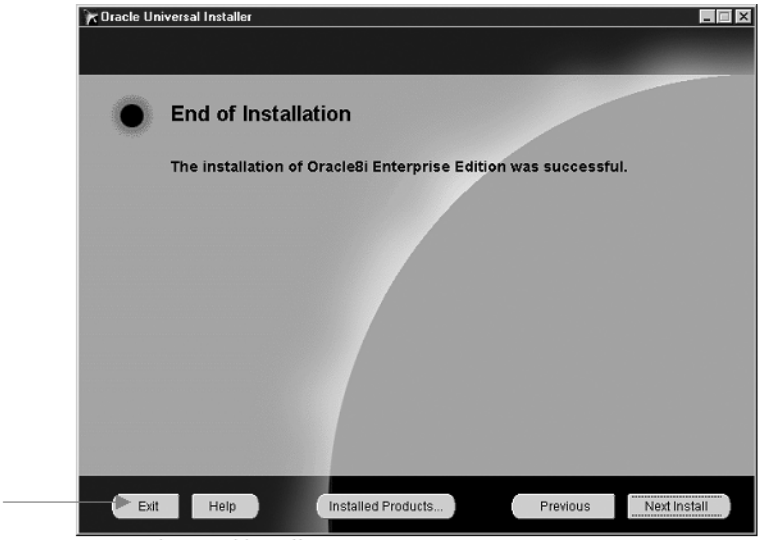
Database creation completed.

Database Information:

global database name: dbstrack
database system identifier (SID): dbstrack
SYS account password: change_on_install
SYSTEM account password: manager

Press OK to end installation

Figure 25.10.End of Installation Window



End of Installation

The installation of Oracle8i Enterprise Edition was successful.

Press exit to end installer

Press Exit to close the installer.

Installing Oracle 8.1.7. Client on a Windows PC 25.3

Figure 25.11.The Install Window

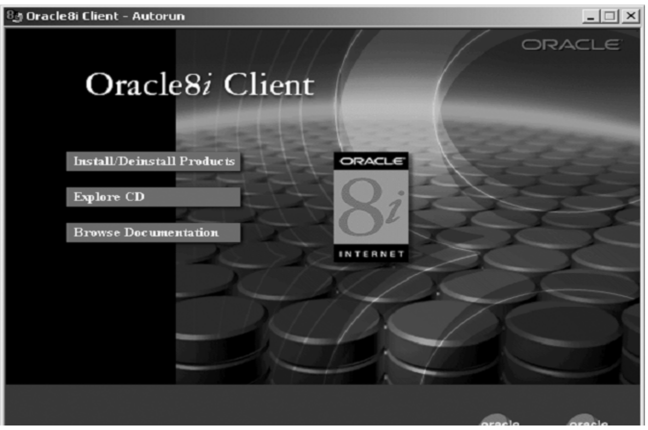
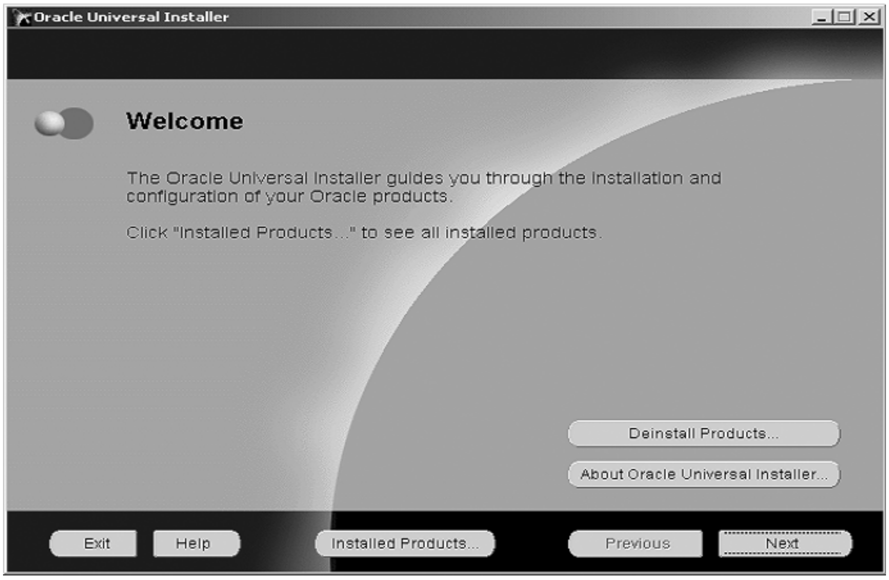


Figure 25.12.Welcome Window



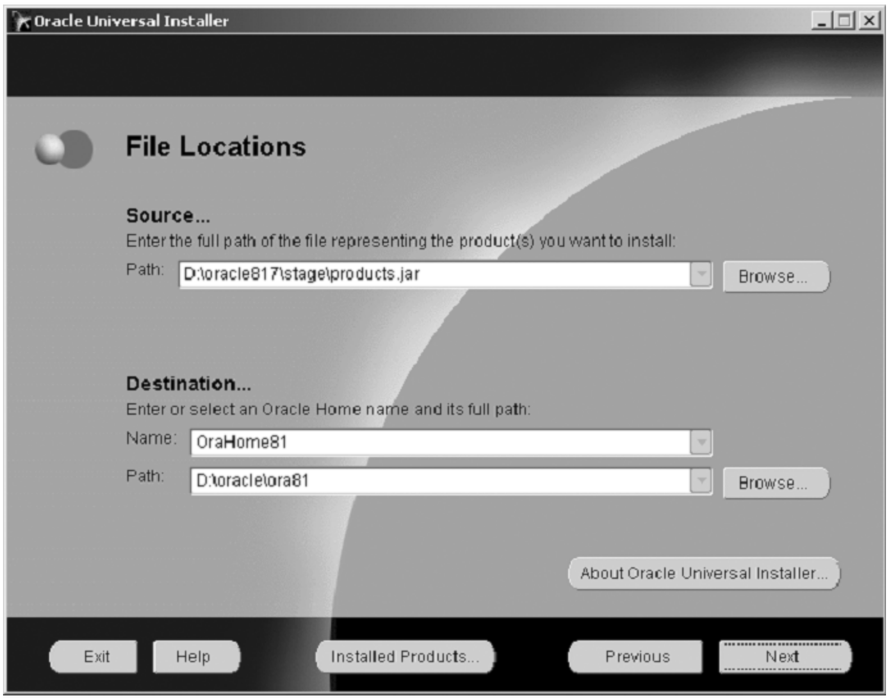
Welcome

The Oracle Universal Installer guides you through the installation and configuration of your Oracle products.

Click "Installed Products..." to see all installed products.

Press **Next**

Figure 25.13.File Location Window


Oracle Universal Installer
Browse...
Browse...
About Oracle Universal Installer...
Exit
Help
Installed Products...
Previous
Next

File Locations

Source...

Enter the full path of the file representing the product(s) you want to install:

Path: D:\oracle817\stage\products.jar

Destination...

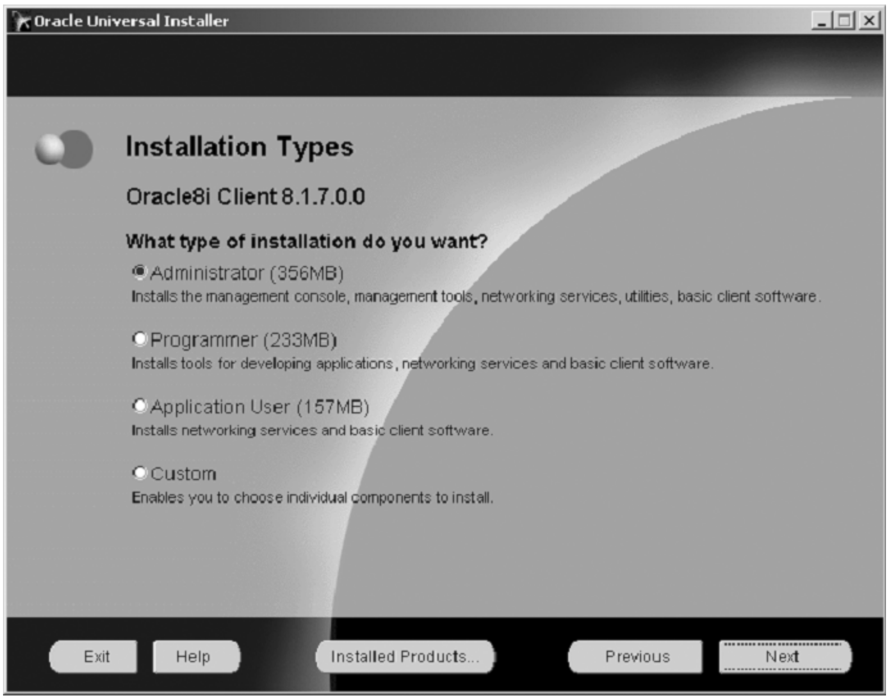
Enter or select an Oracle Home name and its full path:

Name: OraHome81

Path: D:\oracle\ora81

Select the source and destination, then press **Next**

Figure 25.14.Installation Types Window



Installation Types

Oracle8i Client 8.1.7.0.0

What type of installation do you want?

● Administrator (356MB)
Installs the management console, management tools, networking services, utilities, basic client software.

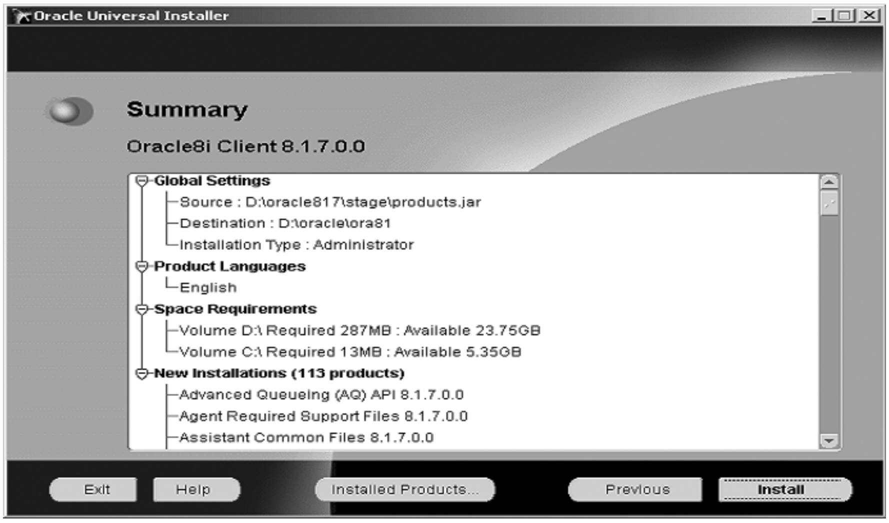
○ Programmer (233MB)
Installs tools for developing applications, networking services and basic client software.

○ Application User (157MB)
Installs networking services and basic client software.

○ Custom
Enables you to choose individual components to install.

Select either „Administrator“ or „Application User“, press **Next**

Figure 25.15.Summary Window



Summary

Oracle8i Client 8.1.7.0.0

Global Settings
- Source : D:\oracle817\stage\products.jar
- Destination : D:\oracle\ora81
- Installation Type : Administrator

Product Languages
- English

Space Requirements
- Volume D:\ Required 287MB : Available 23.75GB
- Volume C:\ Required 13MB : Available 5.35GB

New Installations (113 products)
- Advanced Queueing (AQ) API 8.1.7.0.0
- Agent Required Support Files 8.1.7.0.0
- Assistant Common Files 8.1.7.0.0

A summary of the programes to be installed is shown.

Press **Install** to start the installation.

...

Press **OK** to end installation.

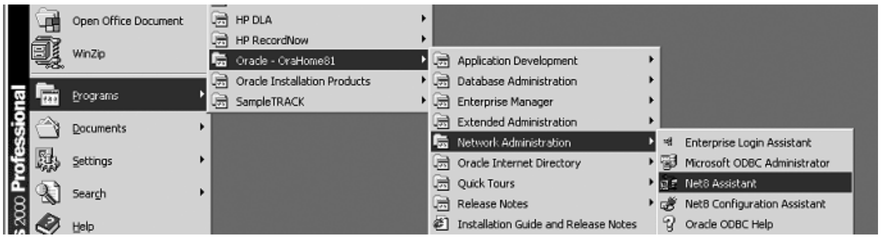
Client/Server Network Connection

26

Net8 Assistant 26.1

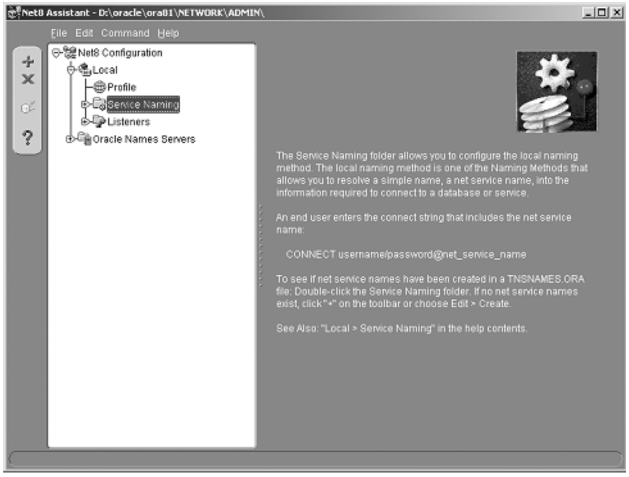
There are several possibilities in creating client/server network connections

Figure 26.1. Client Server Network Connection



The best one is the Net8 Assistant.

Figure 26.2. Service Naming



The Service Naming folder allows you to configure the local naming method. The local naming method is one of the Naming Methods that allows you to resolve a simple name, a net service name, into the information required to connect to a database or service.

An end user enters the connect string that includes the net service name:

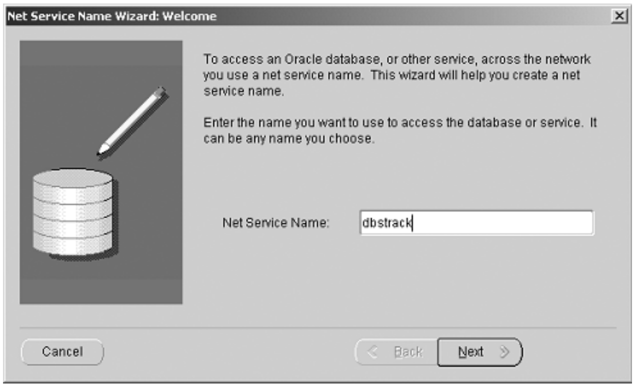
```
CONNECT username/password@net_service_name
```

To see if net service names have been created in a TNSNAMES.ORA file: Double-click the Service Naming folder. If no net service names exist, click "+" on the toolbar or choose Edit > Create.

See Also: "Local > Service Naming" in the help contents.

Mark „Local/Service Naming“ and click the plus symbol.

Figure 26.3. Net Service Name Window



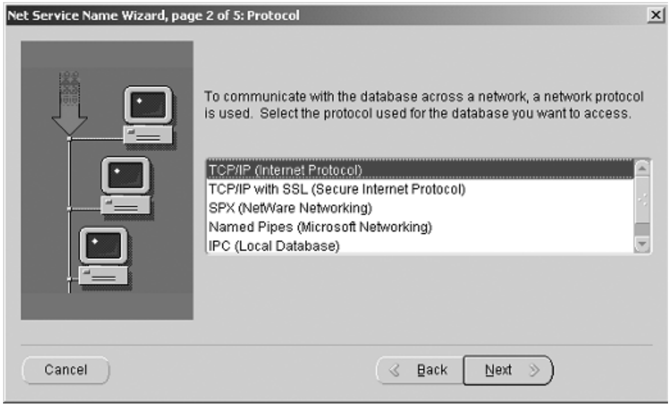
To access an Oracle database, or other service, across the network you use a net service name. This wizard will help you create a net service name.

Enter the name you want to use to access the database or service. It can be any name you choose.

Net Service Name: dbstrack

Enter the netservice name „dbstrack“.

Figure 26.4. Protocol Window

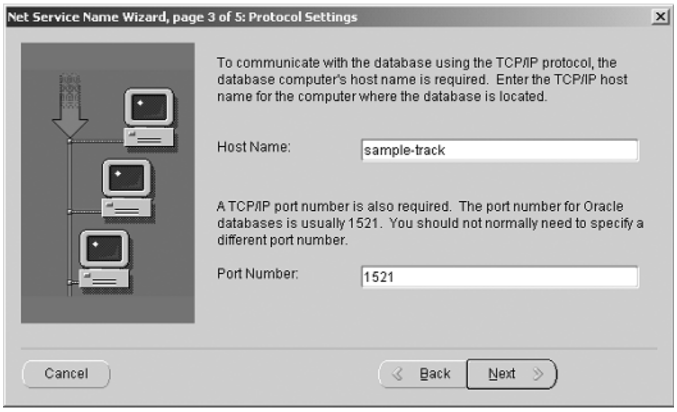


To communicate with the database across a network, a network protocol is used. Select the protocol used for the database you want to access.

- TCP/IP (Internet Protocol)
- TCP/IP with SSL (Secure Internet Protocol)
- SPX (NetWare Networking)
- Named Pipes (Microsoft Networking)
- IPC (Local Database)

Select the network protocol TCP/IP.

Figure 26.5. Host Name Window



To communicate with the database using the TCP/IP protocol, the database computer's host name is required. Enter the TCP/IP host name for the computer where the database is located.

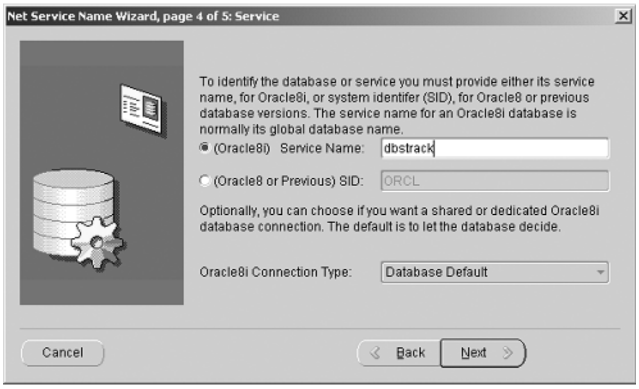
Host Name: sample-track

A TCP/IP port number is also required. The port number for Oracle databases is usually 1521. You should not normally need to specify a different port number.

Port Number: 1521

Enter the host name of the computer where the Oracle Database has been installed.

Figure 26.6. Service Name Window



To identify the database or service you must provide either its service name, for Oracle8i, or system identifer (SID), for Oracle8 or previous database versions. The service name for an Oracle8i database is normally its global database name.

● (Oracle8i) Service Name: dbstrack

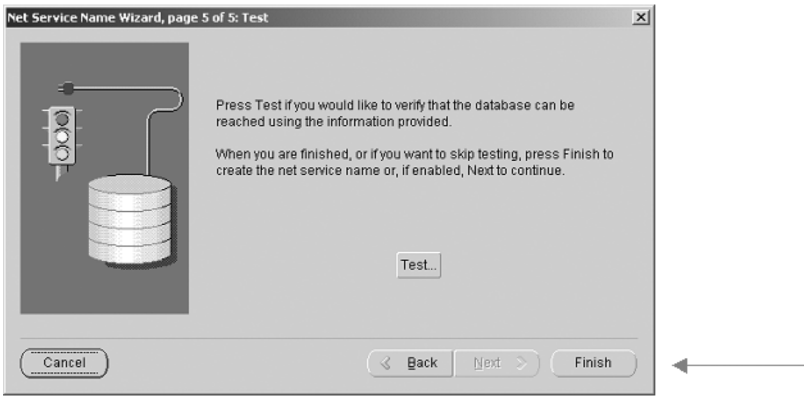
○ (Oracle8 or Previous) SID: ORCL

Optionally, you can choose if you want a shared or dedicated Oracle8i database connection. The default is to let the database decide.

Oracle8i Connection Type: Database Default

For Oracle 8.1.7 or higher use the Oracle 8i Service Name: „dbstrack“

Figure 26.7. Test Window

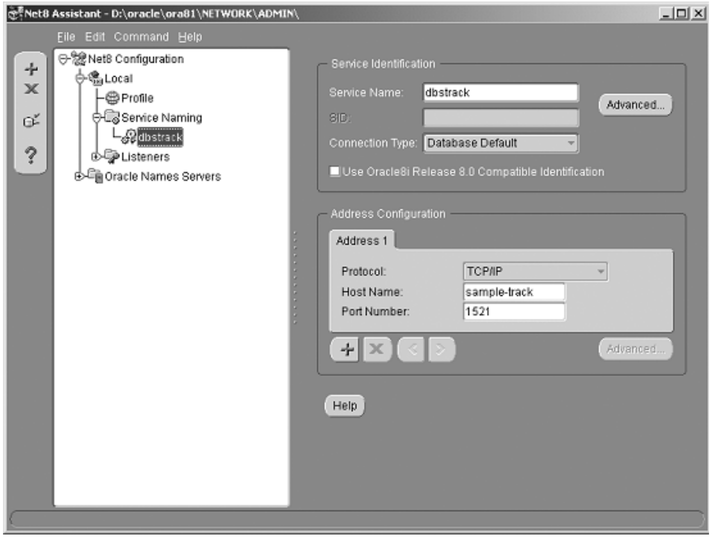


Press Test if you would like to verify that the database can be reached using the information provided.

When you are finished, or if you want to skip testing, press Finish to create the net service name or, if enabled, Next to continue.

Press **Finish** to finish the installation.

Figure 26.8. Result Window



Service Name: dbstrack

SID:

Connection Type: Database Default

☐ Use Oracle8i Release 8.0 Compatible Identification

Protocol: TCP/IP

Host Name: sample-track

Port Number: 1521

After pressing **Finish** the results should look like those above.

SampleTrack™ System and Client Installation

27

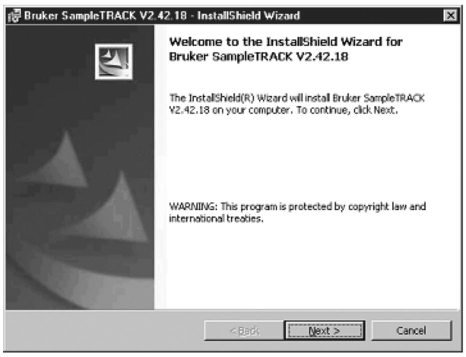
SampleTrack™ System vs. SampleTrack™ Client 27.1

There are only a few differences between the SampleTrack™ System and the SampleTrack™ Client Installation. With the system installation the SampleTrack Communicator moves to the Autostart folder and starts automatically with each PC start. The Communicator often runs on a PC where the database was installed. The PC running the Communicator must have network connection to the database and to all served spectrometer PC's. ST Config is an additional program for the administrator that controls basic connectivity parameters ***"ST Config - A Program for the Administrator" on page 214***.

Figure 27.1. The SampleTrack Installation CD

Figure 27.2. The SampleTrack Installation Wizard

Run the installation program for SampleTrack called
“st**inst**XXX_XX.exe” which is placed on the SampleTrack-CD.
(The actual setup file is named: “st**inst**242_18.exe”)



Bruker SampleTRACK V2.42.18 - InstallShield Wizard

Welcome to the InstallShield Wizard for Bruker SampleTRACK V2.42.18

The InstallShield(R) Wizard will install Bruker SampleTRACK V2.42.18 on your computer. To continue, click Next.

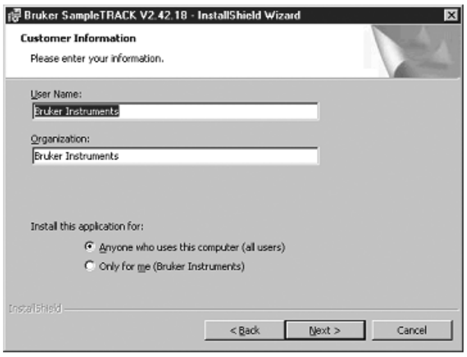
WARNING: This program is protected by copyright law and international treaties.

Run the SampleTrack installation program „stinstXXX_XX.exe“ which is located on the SampleTrack CD.

Press Next to continue.

Enter the customer user name and organization as shown in the figure below:

Figure 27.3. Customer Information Window



Bruker SampleTRACK V2.42.18 - InstallShield Wizard

Customer Information

Please enter your information.

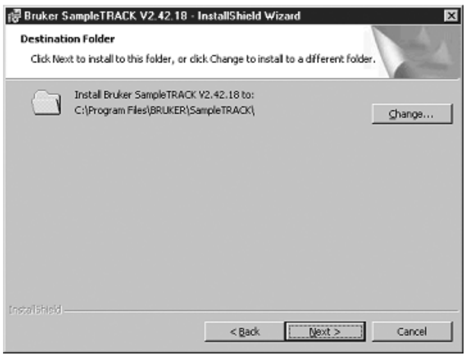
User Name: Bruker Instruments

Organization: Bruker Instruments

Install this application for:

● Anyone who uses this computer (all users)

○ Only for me (Bruker Instruments)



Bruker SampleTRACK V2.42.18 - InstallShield Wizard

Destination Folder

Click Next to install to this folder, or click Change to install to a different folder.

Install Bruker SampleTRACK V2.42.18 to:
C:\Program Files\BRUKER\SampleTRACK\

Enter user name and organization.

Select installation option.

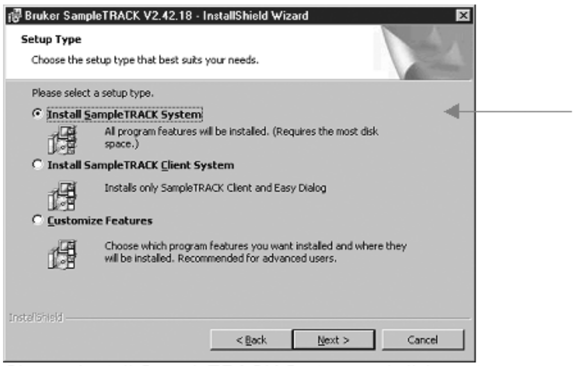
Press Next.

Change destination folder if required.

Press Next.

Choose **Install SampleTrack System** and press **Next**

Figure 27.4. Setup Type Window



Bruker SampleTRACK V2.42.18 - InstallShield Wizard

Setup Type

Choose the setup type that best suits your needs.

Please select a setup type.

● **Install SampleTRACK System**

All program features will be installed. (Requires the most disk space.)

○ **Install SampleTRACK Client System**

Installs only SampleTRACK Client and Easy Dialog

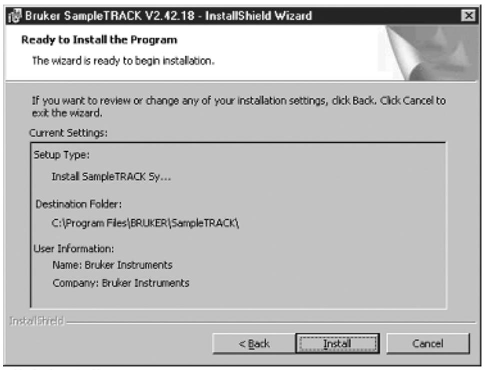
○ **Customize Features**

Choose which program features you want installed and where they will be installed. Recommended for advanced users.

Choose Install SampleTRACK System and click next

Ready to install SampleTrack

Figure 27.5. Installation Overview Window



Bruker SampleTRACK V2.42.18 - InstallShield Wizard

Ready to Install the Program

The wizard is ready to begin installation.

If you want to review or change any of your installation settings, click Back. Click Cancel to exit the wizard.

Current Settings:

Setup Type:
Install SampleTRACK Sy...

Destination Folder:
C:\Program Files\BRUKER\SampleTRACK\

User Information:
Name: Bruker Instruments
Company: Bruker Instruments

click install

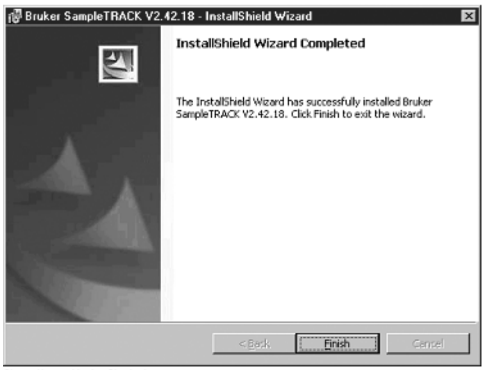
Press Install.

Wait... .

Finish the InstallShield Wizard

Figure 27.6. InstallShield Wizard Completion Window

please wait..



Bruker SampleTRACK V2.42.18 - InstallShield Wizard

InstallShield Wizard Completed

The InstallShield Wizard has successfully installed Bruker SampleTRACK V2.42.18. Click Finish to exit the wizard.

finally click finish

Press Finish.

SampleTrack™ Patches 27.3

Installing the newest SampleTrack Patch.

SampleTrack patches (stbinxxx_xx.exe) contain all the binary files of a complete SampleTrack installation.

They are usually placed in the directory “C:\Program Files\bruker\SampleTrack\bin\” .

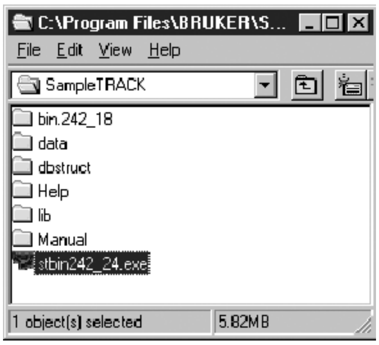
To install the patch copy the file (stbinXXX_XX.exe) to the SampleTrack directory

“C:\Program Files\bruker\SampleTrack\”.

The start the executable file.

The new files will be copied to the ./bin directory. It is allowed to remove, rename or delete the old bin-directory before installing the patch to get rid of any invalid files.

Figure 27.7. Installing the SampleTrack Patch



C:\Program Files\BRUKER\S...

bin.242_18
data
dbstruct
Help
lib
Manual
stbin242_24.exe

1 object(s) selected 5.82MB

The actual SampleTrack patch is also available on the Bruker FTP-server:

ftp://ftp.bruker.de/pub/nmr/SAMTRACK/INSTALL/V2.X

Running SampleTrack™ for the First Time *27.4*

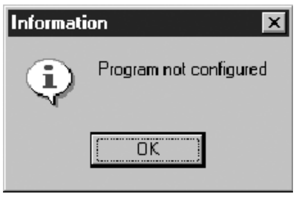
The SampleTrack Client checks the availability and the installation state of the SampleTrack database when it is first run.

In this description the behavior of the SampleTrack client is shown when running the first time on an “empty” Oracle® database.

Such a system is present if Oracle® was installed as described in the first chapter.

If running the SampleTrack client for the first time the following message should appear:

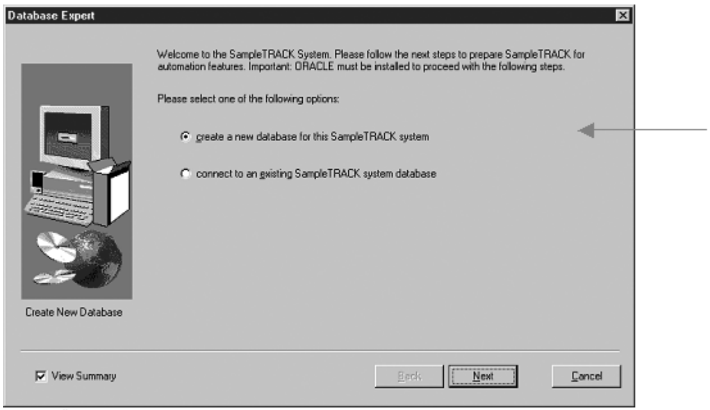
Figure 27.8. Information Window



Program not configured

Press OK.

Figure 27.9. Database Export Window



Welcome to the SampleTRACK System. Please follow the next steps to prepare SampleTRACK for automation features. Important: ORACLE must be installed to proceed with the following steps.

Please select one of the following options:

● create a new database for this SampleTRACK system

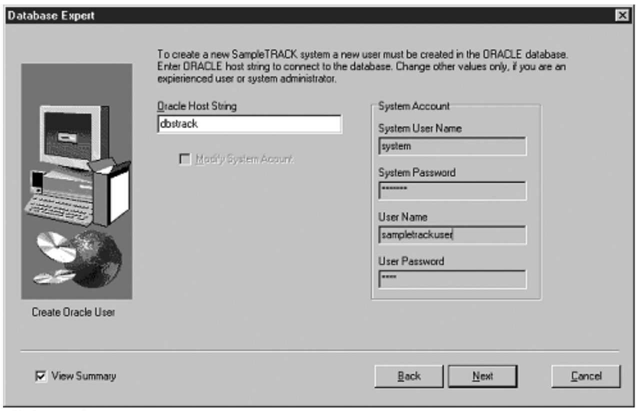
○ connect to an existing SampleTRACK system database

select “create a new database for SampleTrack System” and click next

Select **Create a new database for SampleTrack System** and press Next.

*Enter the Standard Oracle® Host String - **dbstrack***

Figure 27.10.Standard Oracle® Host String



To create a new SampleTRACK system a new user must be created in the ORACLE database. Enter ORACLE host string to connect to the database. Change other values only, if you are an expierienced user or system administrator.

Oracle Host String: dbstrack

System User Name: system

System Password: *******

User Name: sampletrackuser

User Password: ****

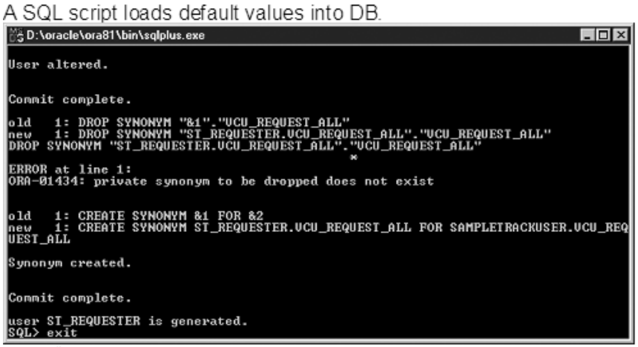
click next

Press **Next.**

A SQL script loads the default values into the database.

Figure 27.11.SQL Script Window

A SQL script loads default values into DB.



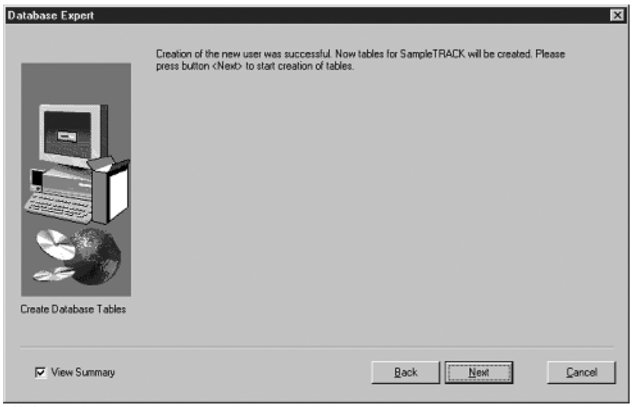
```
User altered.


Commit complete.

old   1: DROP SYNONYM "&1"."VCU_REQUEST_ALL"
new   1: DROP SYNONYM "ST_REQUESTER.VCU_REQUEST_ALL"."VCU_REQUEST_ALL"
DROP SYNONYM "ST_REQUESTER.VCU_REQUEST_ALL"."VCU_REQUEST_ALL"
                                            *
ERROR at line 1:
ORA-01434: private synonym to be dropped does not exist


old   1: CREATE SYNONYM &1 FOR &2
new   1: CREATE SYNONYM ST_REQUESTER.VCU_REQUEST_ALL FOR SAMPLETRACKUSER.VCU_REQ
UEST_ALL

Synonym created.


Commit complete.

user ST_REQUESTER is generated.
SQL> exit
```

enter "exit"

Enter Exit.

When the storage of the standard values was completed successfully the following window will appear:

Figure 27.12.Confirmation Window



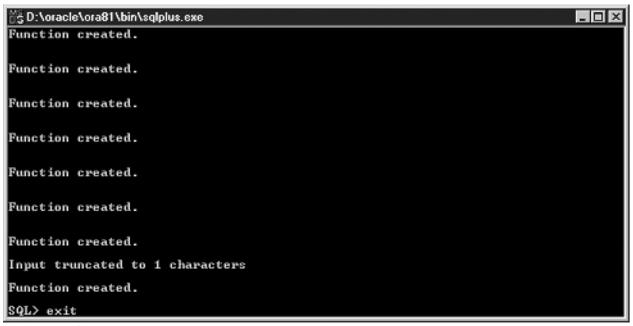
Creation of the new user was successful. Now tables for SampleTRACK will be created. Please press button <Next> to start creation of tables.

☑ View Summary

click next

Press **Next**.

Figure 27.13.Command Prompt Window



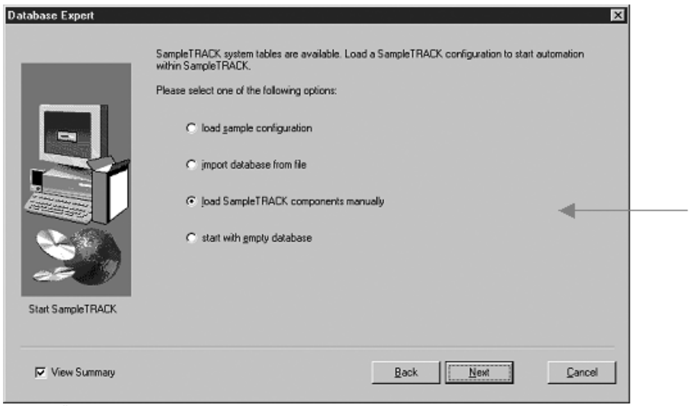
```
Function created.

Function created.

Function created.

Function created.

Function created.

Function created.

Function created.
Input truncated to 1 characters
Function created.
SQL> exit
```

enter exit

Enter **Exit**.

Load SampleTrack components manually

Figure 27.14.Load Components Window



SampleTRACK system tables are available. Load a SampleTRACK configuration to start automation within SampleTRACK.

Please select one of the following options:

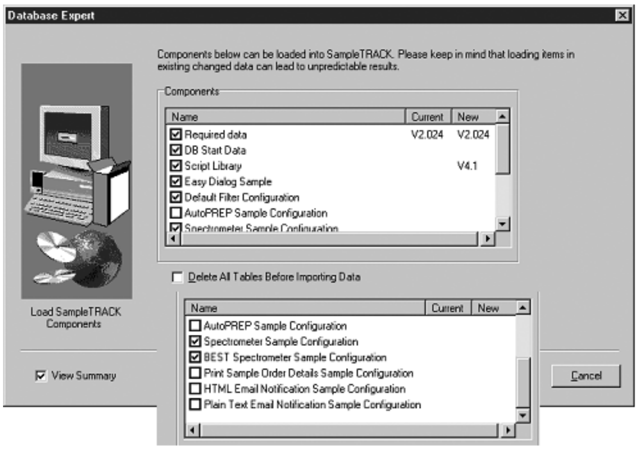
- ○ load sample configuration
- ○ import database from file
- ● load SampleTRACK components manually
- ○ start with empty database

☑ View Summary

select “load SampleTrack components manually” and click next

Select the items that you want installed from the **Component Selection Window**.

Figure 27.15.Component Selection Window



Database Expert

Components below can be loaded into SampleTRACK. Please keep in mind that loading items in existing changed data can lead to unpredictable results.

Components

Name	Current	New
☑ Required data	V2.024	V2.024
☑ DB Start Data		
☑ Script Library		V4.1
☑ Easy Dialog Sample		
☑ Default Filter Configuration		
☐ AutoPREP Sample Configuration		
☑ Spectrometer Sample Configuration		

☐ Delete All Tables Before Importing Data

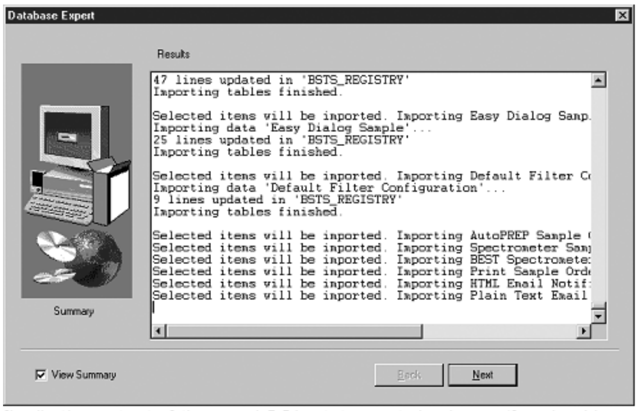
Name	Current	New
☐ AutoPREP Sample Configuration		
☑ Spectrometer Sample Configuration		
☑ BEST Spectrometer Sample Configuration		
☐ Print Sample Order Details Sample Configuration		
☐ HTML Email Notification Sample Configuration		
☐ Plain Text Email Notification Sample Configuration		

select the items as shown

The items selected depend on the user’s instrument environment.

The SQL statements output will be displayed:

Figure 27.16.Output of SQL Statements



Database Expert

Results

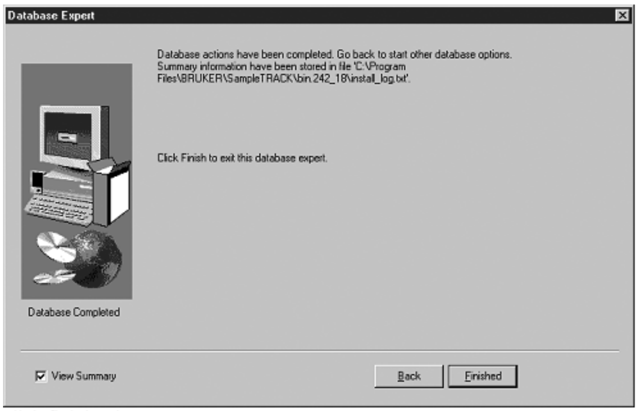
```
47 lines updated in 'BSTS_REGISTRY'
Importing tables finished.

Selected items will be imported. Importing Easy Dialog Samp.
Importing data 'Easy Dialog Sample'...
25 lines updated in 'BSTS_REGISTRY'
Importing tables finished.

Selected items will be imported. Importing Default Filter C
Importing data 'Default Filter Configuration'...
9 lines updated in 'BSTS_REGISTRY'
Importing tables finished.

Selected items will be imported. Importing AutoPREP Sample
Selected items will be imported. Importing Spectrometer Sam
Selected items will be imported. Importing BEST Spectromete
Selected items will be imported. Importing Print Sample Ord
Selected items will be imported. Importing HTML Email Notif
Selected items will be imported. Importing Plain Text Email
```

finally the output of the used SQL-statements is shown (for checking only)
click next

Press Next.

This completes the database installation.

Figure 27.17.Program Completion Window



Database Expert

Database actions have been completed. Go back to start other database options. Summary information have been stored in file 'C:\Program Files\BRUKER\SampleTRACK\bin.242_18\install_log.txt'.

Click Finish to exit this database expert.

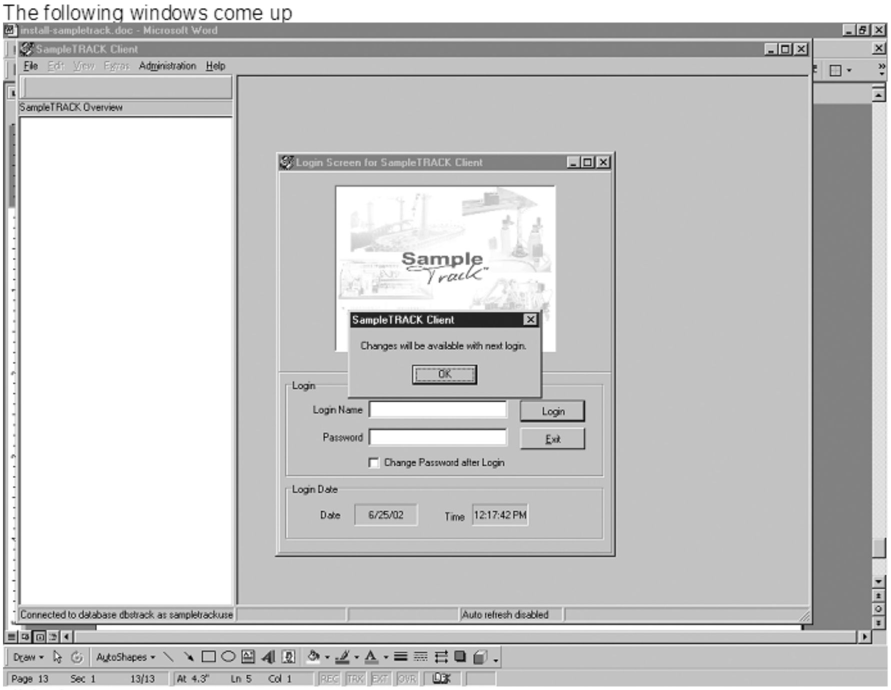
click finished

Press Finished.

The changes will be available with the next login.

Figure 27.18.Change Completion Verification Window

The following windows come up



SampleTRACK Client

Changes will be available with next login.

Login Date

Date 6/25/02

Time 12:17:42 PM

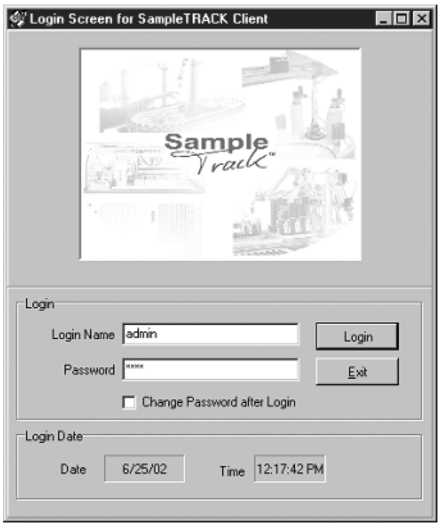
Connected to database dbstrack as sampletrackuse

Auto refresh disabled

click ok

Press **OK**.

Figure 27.19.The Login Window



Login Name admin

Password ****

☐ Change Password after Login

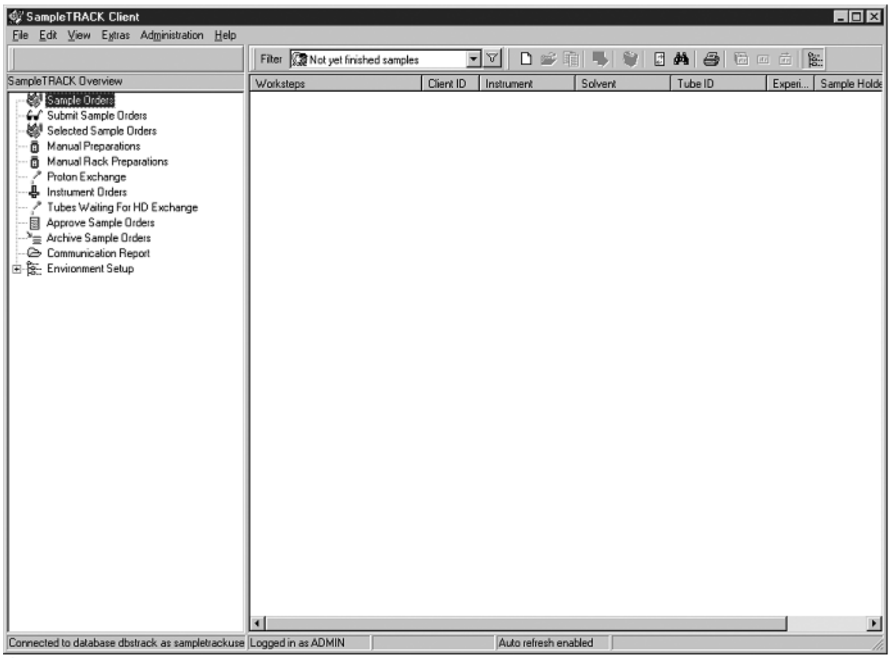
Date 6/25/02

Time 12:17:42 PM

login

This completes the procedure.

Figure 27.20.The SampleTrack Client Window



Filter Not yet finished samples

Connected to database dbstrack as sampletrackuse

Logged in as ADMIN

Auto refresh enabled

done

SampleTrack™ Program Icons 27.5

After the system restart the following new entries will be found:

Figure 27.21.SampleTrack Program Icons

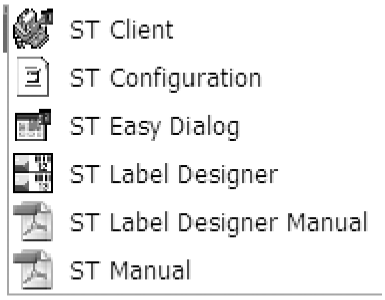
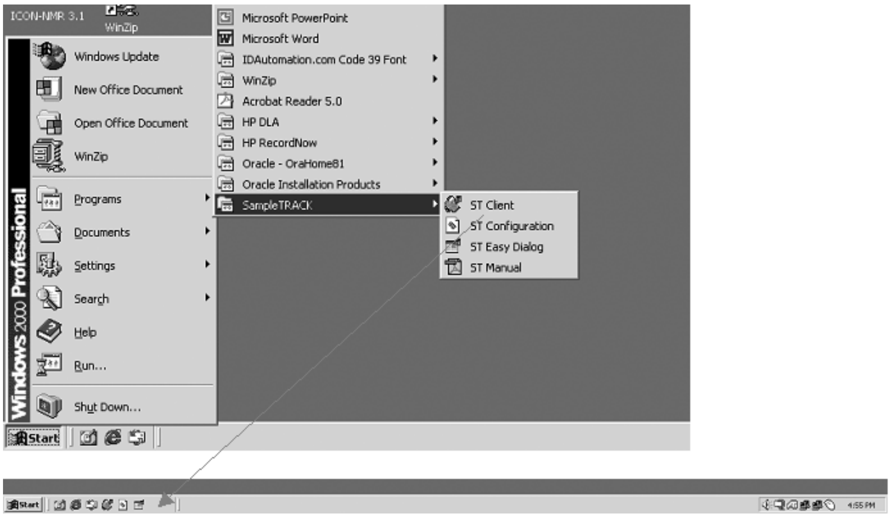


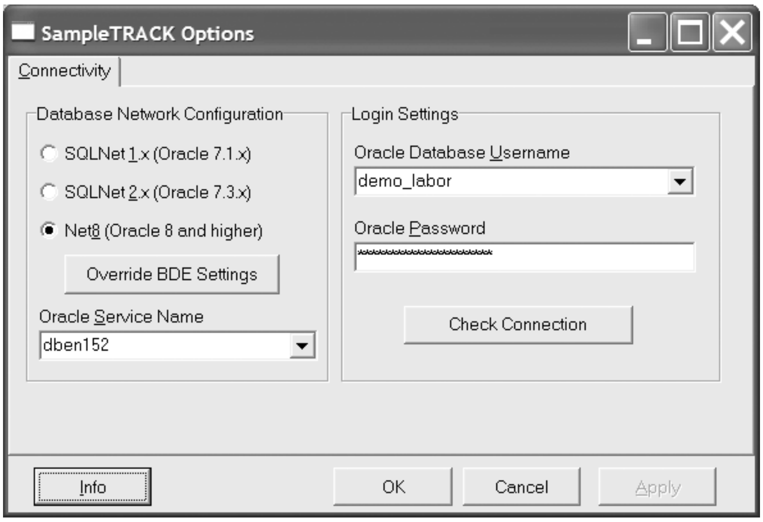
Figure 27.22.The Toolbar



It is recommended that you place the icons ST Client and ST EasyDialog for each user into the toolbar by pressing theControl key and moving the icon.

The program ST Configuration tool is meant for use by the administrator only.

Figure 27.23.The ST Config Window


SampleTRACK Options
Connectivity
Database Network Configuration
○ SQLNet 1.x (Oracle 7.1.x)
○ SQLNet 2.x (Oracle 7.3.x)
● Net8 (Oracle 8 and higher)
Override BDE Settings
Login Settings
Check Connection
Info
OK
Cancel
Apply

Oracle Service Name: dben152

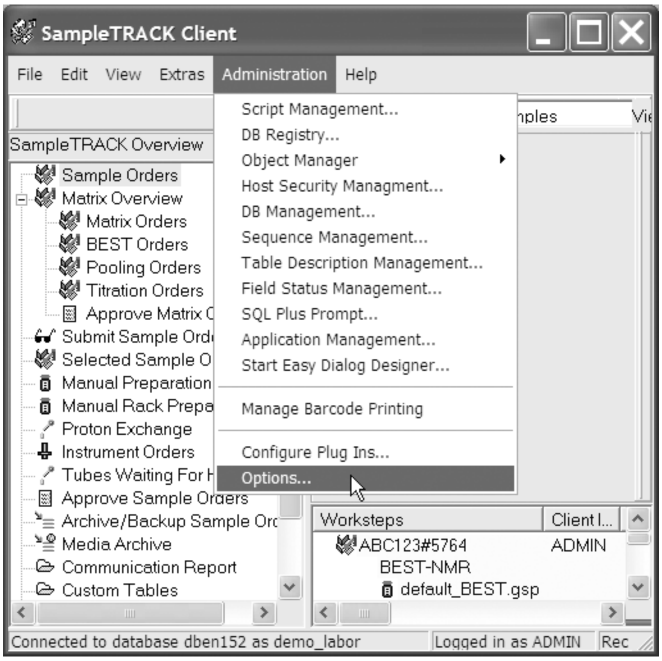
Oracle Database Username: demo_labor

Oracle Password: ********************

Important connectivity settings are set in this stand-alone program. It is identical to the tab of the SampleTrack options found within the client menu - **Administration - SampleTrack Options - Tab Connectivity.**

The entries here play a role when a database connection error occurs after the installation.

Figure 27.24.The SampleTrack Administration Menu Option



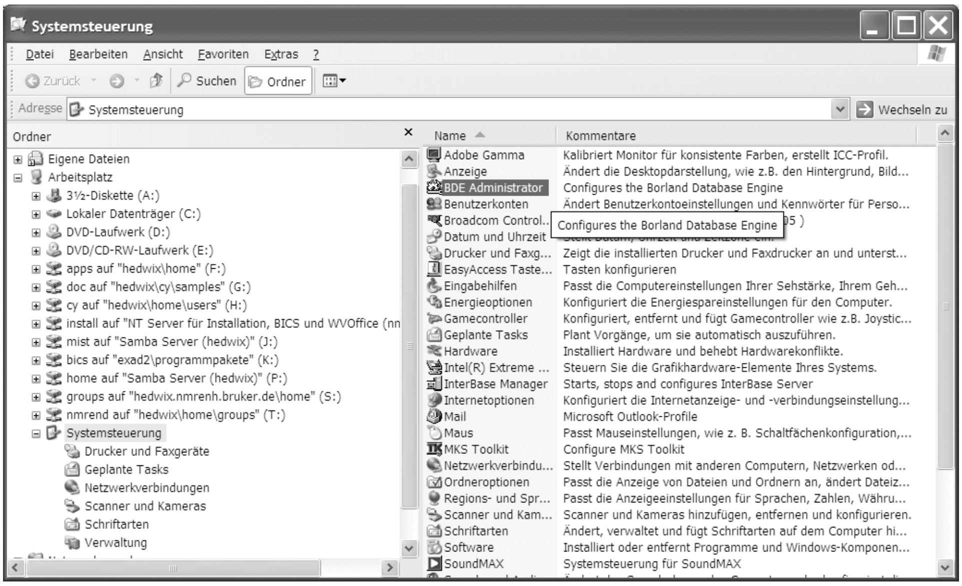
Connected to database dben152 as demo_labor | Logged in as ADMIN | Rec

Database Connection Error After New Installation 27.7

This is a common problem with the BORLAND® BDE (Borland® Database Engine). The easiest way to handle the connectivity settings is by clicking the button **Override BDE Settings** see the figure ***"The ST Config Window" on page 214*** within the SampleTrack Connectivity window - either within the ST Configuration program or under SampleTrack client - Administration - Options.

You can also change the BDE settings in the control panel

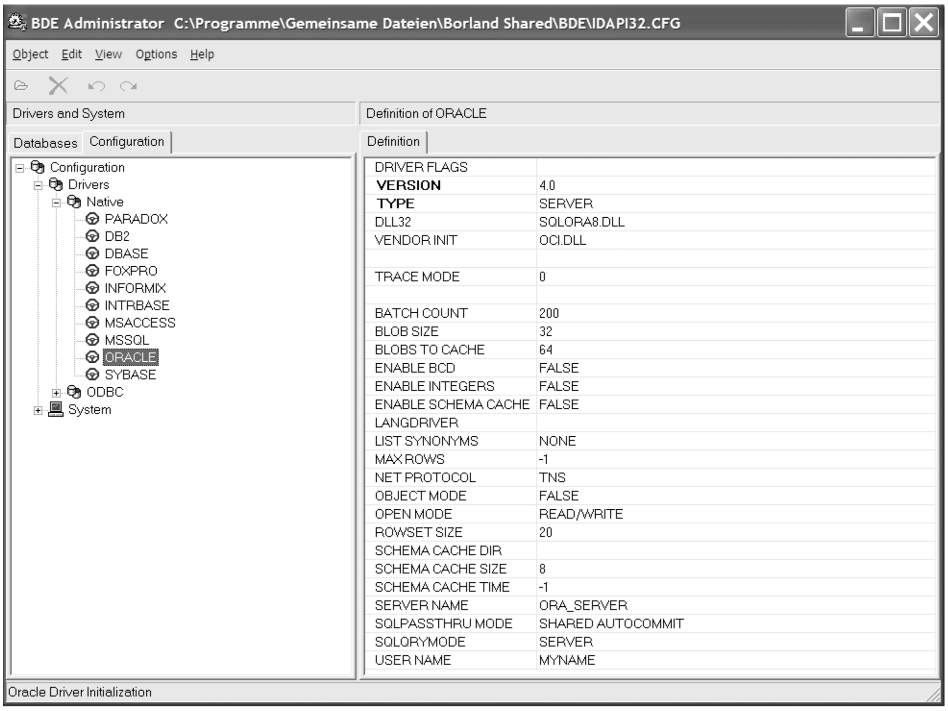
Figure 27.25.BDE Administrator Window


Systemsteuerung
Datei Bearbeiten Ansicht Favoriten Extras ?
Zurück
Suchen
Ordner
Adresse
Systemsteuerung
Wechseln zu
Ordner
Eigene Dateien
Arbeitsplatz
3½-Diskette (A:)
Lokaler Datenträger (C:)
DVD-Laufwerk (D:)
DVD/CD-RW-Laufwerk (E:)
apps auf "hedwix\home" (F:)
doc auf "hedwix\cy\samples" (G:)
cy auf "hedwix\home\users" (H:)
install auf "NT Server für Installation, BICS und WVOffice (nn
mist auf "Samba Server (hedwix)" (J:)
bics auf "exad2\programmpakete" (K:)
home auf "Samba Server (hedwix)" (P:)
groups auf "hedwix.nmrenh.bruker.de\home" (S:)
nmrend auf "hedwix\home\groups" (T:)
Systemsteuerung
Drucker und Faxgeräte
Geplante Tasks
Netzwerkverbindungen
Scanner und Kameras
Schriftarten
Verwaltung
Configures the Borland Database Engine

Name	Kommentare
Adobe Gamma	Kalibriert Monitor für konsistente Farben, erstellt ICC-Profil.
Anzeige	Ändert die Desktopdarstellung, wie z.B. den Hintergrund, Bild...
BDE Administrator	Configures the Borland Database Engine
Benutzerkonten	Ändert Benutzerkontoeinstellungen und Kennwörter für Perso...
Broadcom Control...	05)
Datum und Uhrzeit	Stellt Datum, Uhrzeit und Zeitzone ein.
Drucker und Faxg...	Zeigt die installierten Drucker und Faxdrucker an und unterst...
EasyAccess Taste...	Tasten konfigurieren
Eingabehilfen	Passt die Computereinstellungen Ihrer Sehstärke, Ihrem Geh...
Energieoptionen	Konfiguriert die Energiespareinstellungen für den Computer.
Gamecontroller	Konfiguriert, entfernt und fügt Gamecontroller wie z.B. Joystic...
Geplante Tasks	Plant Vorgänge, um sie automatisch auszuführen.
Hardware	Installiert Hardware und behebt Hardwarekonflikte.
Intel(R) Extreme ...	Steuern Sie die Grafikhardware-Elemente Ihres Systems.
InterBase Manager	Starts, stops and configures InterBase Server
Internetoptionen	Konfiguriert die Internetanzeige- und -verbindungseinstellung...
Mail	Microsoft Outlook-Profile
Maus	Passt Mauseinstellungen, wie z. B. Schaltfächenkonfiguration,...
MKS Toolkit	Configure MKS Toolkit
Netzwerkverbindu...	Stellt Verbindungen mit anderen Computern, Netzwerken od...
Ordneroptionen	Passt die Anzeige von Dateien und Ordnern an, ändert Dateiz...
Regions- und Spr...	Passt die Anzeigeeinstellungen für Sprachen, Zahlen, Währu...
Scanner und Kam...	Scanner und Kameras hinzufügen, entfernen und konfigurieren.
Schriftarten	Ändert, verwaltet und fügt Schriftarten auf dem Computer hi...
Software	Installiert oder entfernt Programme und Windows-Komponen...
SoundMAX	Systemsteuerung für SoundMAX

On the tab Configuration - Drivers - Native - ORACLE change the entry in the ORACLE definition window DLL32 to „SQLORA8.DLL“ and the VENDOR INIT to „OCI.DLL“.

Figure 27.26.BDE Administrator Window: DLL32 and VENDOR INIT



DRIVER FLAGS	
VERSION	4.0
TYPE	SERVER
DLL32	SQLORA8.DLL
VENDOR INIT	OCI.DLL
TRACE MODE	0
BATCH COUNT	200
BLOB SIZE	32
BLOBS TO CACHE	64
ENABLE BCD	FALSE
ENABLE INTEGERS	FALSE
ENABLE SCHEMA CACHE	FALSE
LANGDRIVER	
LIST SYNONYMS	NONE
MAX ROWS	-1
NET PROTOCOL	TNS
OBJECT MODE	FALSE
OPEN MODE	READ/WRITE
ROWSET SIZE	20
SCHEMA CACHE DIR	
SCHEMA CACHE SIZE	8
SCHEMA CACHE TIME	-1
SERVER NAME	ORA_SERVER
SQLPASSTHRU MODE	SHARED AUTOCOMMIT
SQLQRYMODE	SERVER
USER NAME	MYNAME

Apply your changes and login to the SampleTrack Client.

Installation of Instruments *27.8*

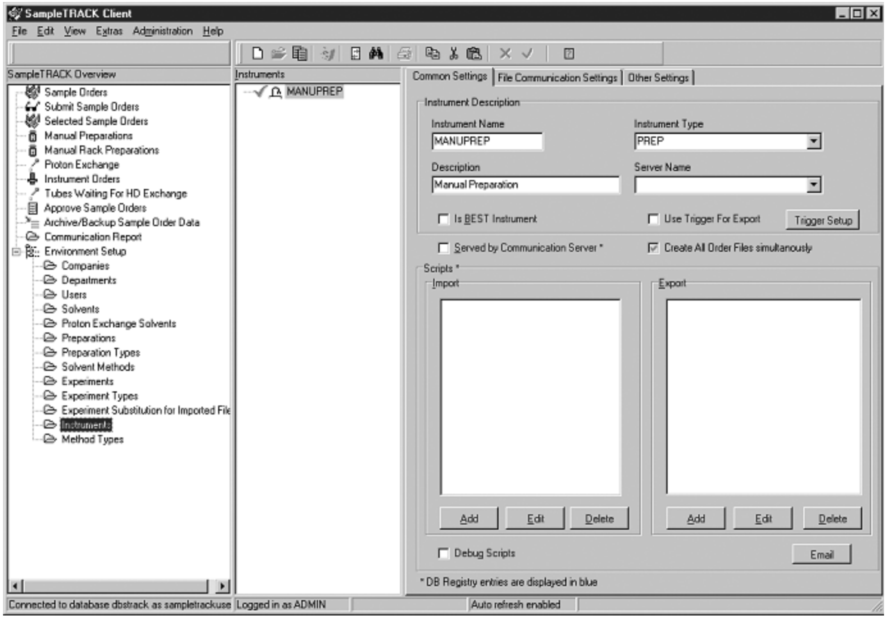
This section describes how to install the different types of instruments.

SampleTrack supported instruments include:

- NMR spectrometer using BACS with barcoded tubes
- NMR spectrometer with BEST and barcoded Gilson racks
- Bruker AutoPrep (ASP)
- Gilson Preparation Robots controlled by BRUKER software
- Other Preparation Robots using the provided interface
- Bruker SampleRail™ System
- Interfaces to other data management systems

The Environment Setup Window shows the installed instruments.

Figure 27.27.Environment Setup Window



Instrument Name: MANUPREP
Instrument Type: PREP
Description: Manual Preparation
Server Name:

☐ Is BEST Instrument
☐ Use Trigger For Export
☐ Served by Communication Server *
☑ Create All Order Files simultanously
☐ Debug Scripts

* DB Registry entries are displayed in blue

Connected to database dbstrack as sampletrackuse | Logged in as ADMIN | Auto refresh enabled

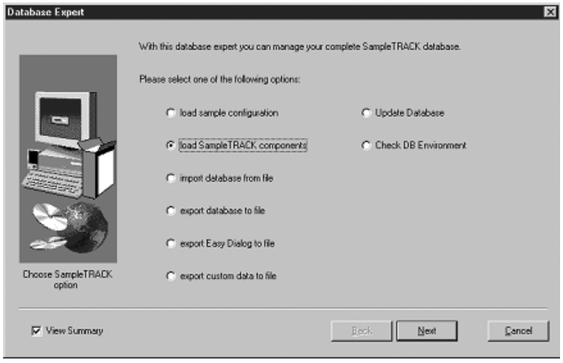
The only instrument installed here is called MANUPREP which symbolizes the manual preparation work center.

Installation of BRUKER NMR Spectrometer Using B-ACS 27.9

1. Installation of a Dummy Instrument from a Template. 27.9.1

- Open the SampleTrack client
- Select menu point Administration – DB Management

Figure 27.28.The Load SampleTrack Components Window



With this database expert you can manage your complete SampleTRACK database.

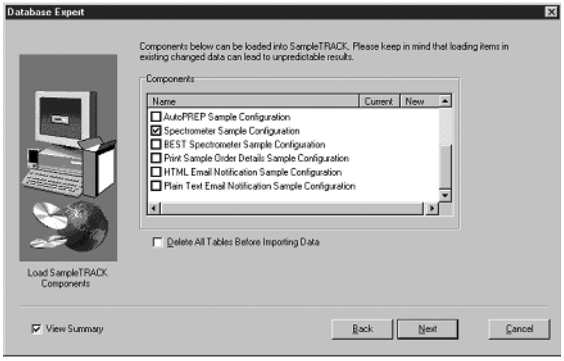
Please select one of the following options:

○ load sample configuration
● load SampleTRACK components
○ import database from file
○ export database to file
○ export Easy Dialog to file
○ export custom data to file
○ Update Database
○ Check DB Environment

☑ View Summary

Choose **Load SampleTrack Components** and press **Next**.

Figure 27.29.Spectrometer Configuration Window



Components below can be loaded into SampleTRACK. Please keep in mind that loading items in existing changed data can lead to unpredictable results.

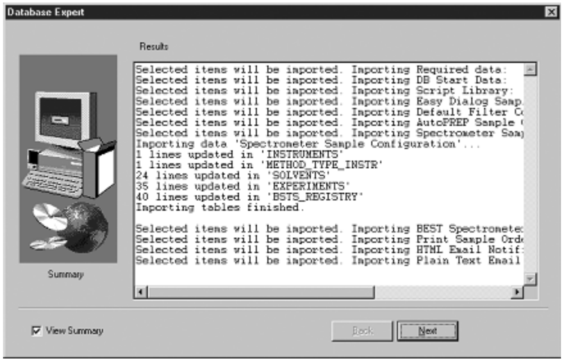
- ☐ AutoPREP Sample Configuration
- ☑ Spectrometer Sample Configuration
- ☐ BEST Spectrometer Sample Configuration
- ☐ Print Sample Order Details Sample Configuration
- ☐ HTML Email Notification Sample Configuration
- ☐ Plain Text Email Notification Sample Configuration

☐ Delete All Tables Before Importing Data

☑ View Summary

Select **Spectrometer Sample Configuration** and Press **Next**.

Figure 27.30.SQL Output Window



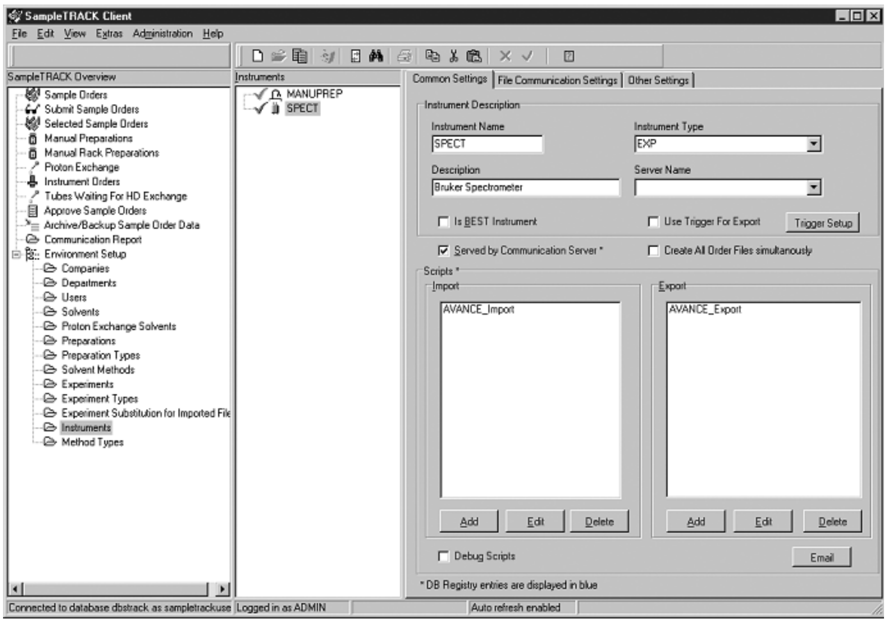
```
Selected items will be imported. Importing Required data:
Selected items will be imported. Importing DB Start Data:
Selected items will be imported. Importing Script Library:
Selected items will be imported. Importing Easy Dialog Samp
Selected items will be imported. Importing Default Filter C
Selected items will be imported. Importing AutoPREP Sample
Selected items will be imported. Importing Spectrometer Sam
Importing data 'Spectrometer Sample Configuration'...
1 lines updated in 'INSTRUMENTS'
1 lines updated in 'METHOD_TYPE_INSTR'
24 lines updated in 'SOLVENTS'
35 lines updated in 'EXPERIMENTS'
40 lines updated in 'BSTS_REGISTRY'
Importing tables finished.

Selected items will be imported. Importing BEST Spectromete
Selected items will be imported. Importing Print Sample Ord
Selected items will be imported. Importing HTML Email Notif
Selected items will be imported. Importing Plain Text Email
```

☑ View Summary

Press **Next**, **Finished** and finally login to SampleTrack client.

Name it in accordance to the spectrometer type (e.g. AV400, AV400_BEST, DPX300_1, DPX300_2, …)

Figure 27.31.The Instrument Setup Window



Instrument Description

Instrument Name: SPECT

Instrument Type: EXP

Description: Bruker Spectrometer

Server Name:

☐ Is BEST Instrument

☐ Use Trigger For Export

☑ Served by Communication Server *

☐ Create All Order Files simultanously

Scripts *

Import: AVANCE_Import

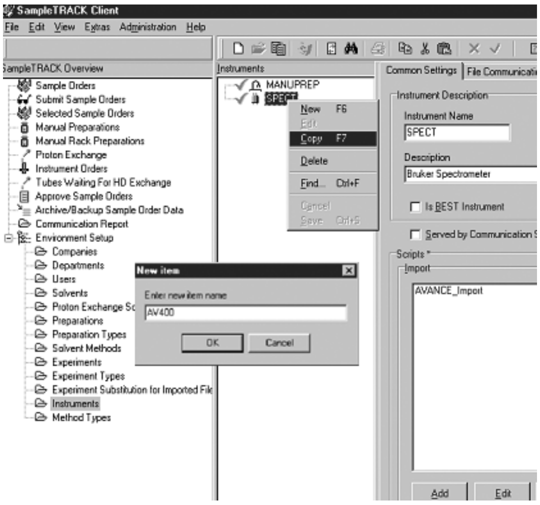
Export: AVANCE_Export

☐ Debug Scripts

* DB Registry entries are displayed in blue

Connected to database dbstrack as sampletrackuse | Logged in as ADMIN | Auto refresh enabled

Figure 27.32.The New Instrument Name Window



New item

Enter new item name: AV400

Instrument Description

Instrument Name: SPECT

Description: Bruker Spectrometer

☐ Is BEST Instrument

☐ Served by Communication S

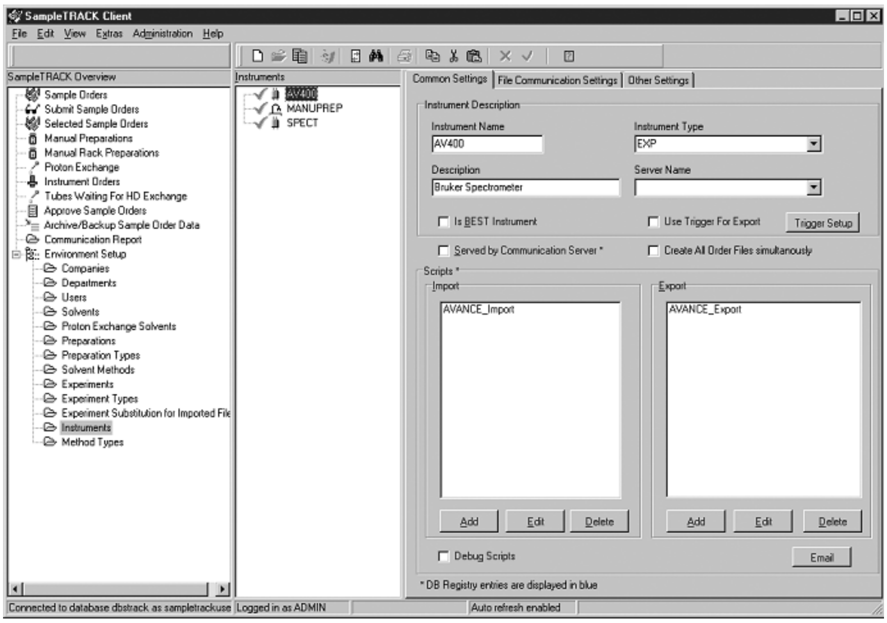
Scripts *

Import: AVANCE_Import

Enter the name of the new intrument (use capital letters) and click OK.Now click on the green check mark to store. The instrument will now appear in the list.

Enter the import and export scripts by clicking the **Add** buttons and select the corresponding script from the list.

Figure 27.33.The Import and Export Scripts Window



Instrument Name: AV400

Instrument Type: EXP

Description: Bruker Spectrometer

Server Name:

☐ Is BEST Instrument

☐ Use Trigger For Export

☐ Served by Communication Server *

☐ Create All Order Files simultanously

Import: AVANCE_Import

Export: AVANCE_Export

☐ Debug Scripts

* DB Registry entries are displayed in blue

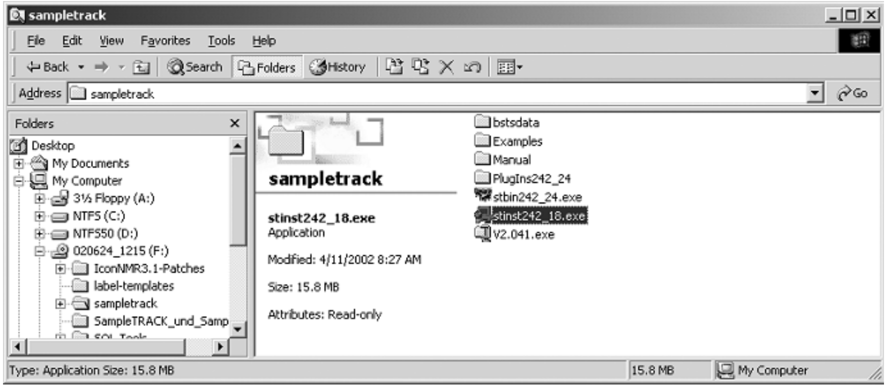
Connected to database dbstrack as sampletrackuse | Logged in as ADMIN | Auto refresh enabled

This completes this procedure.

SampleTrack™ Client Installation 27.10

Install the program stinstxxx_xx.exe from the SampleTrack installer CD.

Figure 27.34.The Explorer Window



sampletrack

stinst242_18.exe
Application

Modified: 4/11/2002 8:27 AM

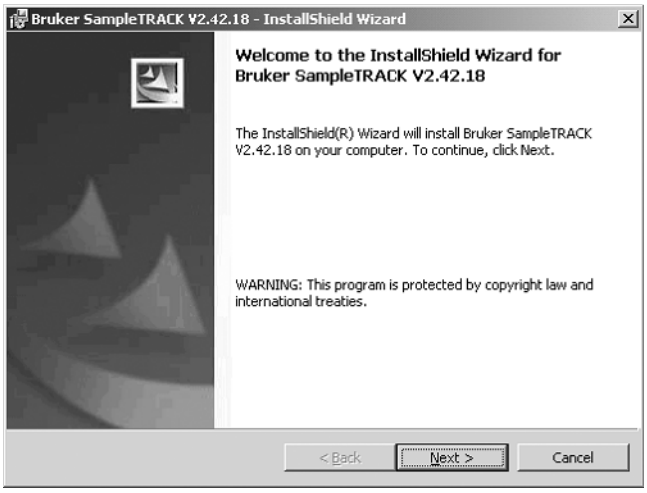
Size: 15.8 MB

Attributes: Read-only

Type: Application Size: 15.8 MB

The InstallShield Wizard will lead you through the installation.

Figure 27.35.InstallShield Wizard Welcome Window



Welcome to the InstallShield Wizard for Bruker SampleTRACK V2.42.18

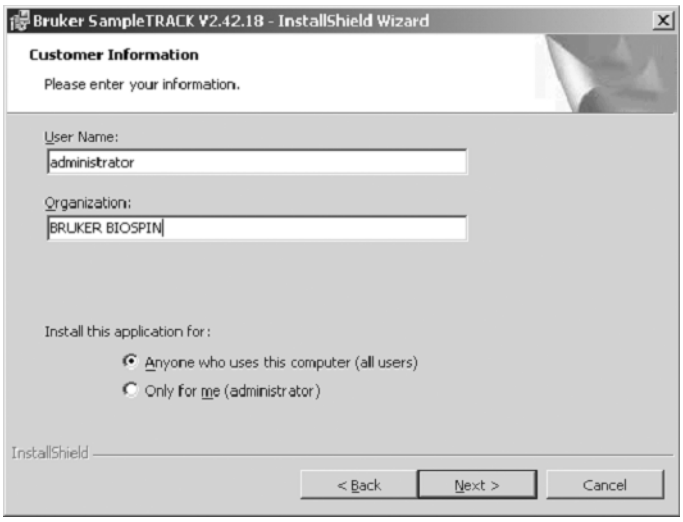
The InstallShield(R) Wizard will install Bruker SampleTRACK V2.42.18 on your computer. To continue, click Next.

WARNING: This program is protected by copyright law and international treaties.

Press **Next**.

Enter your user and company name

Figure 27.36.InstallShield Wizard Window



Bruker SampleTRACK V2.42.18 - InstallShield Wizard

Customer Information

Please enter your information.

User Name: administrator

Organization: BRUKER BIOSPIN

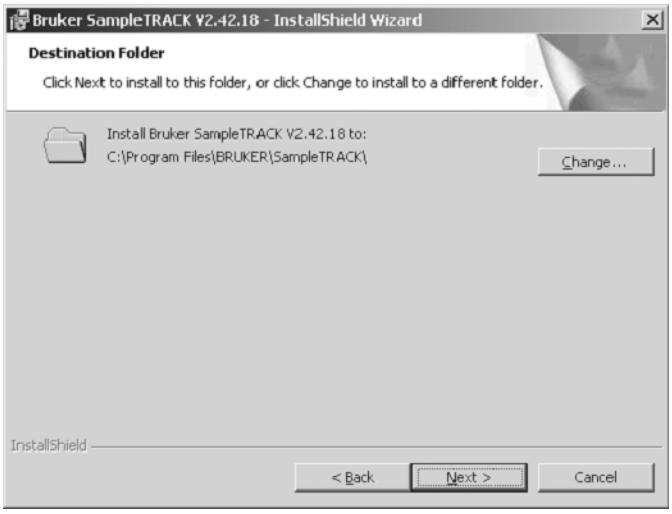
Install this application for:

● Anyone who uses this computer (all users)

○ Only for me (administrator)

Commit or change the default destination folder.

Figure 27.37.The Destination Folder Window



Bruker SampleTRACK V2.42.18 - InstallShield Wizard

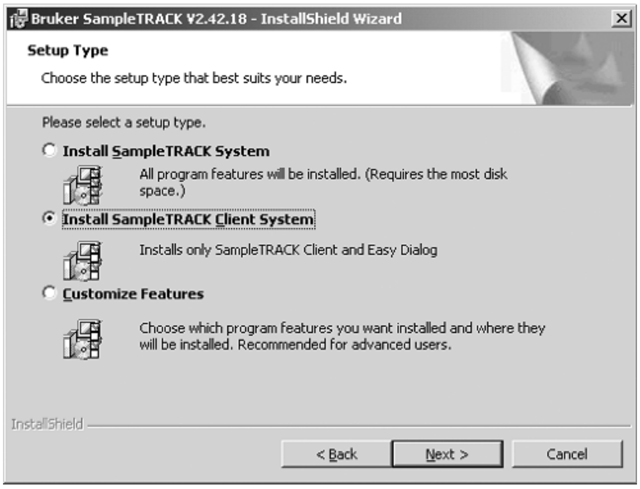
Destination Folder

Click Next to install to this folder, or click Change to install to a different folder.

Install Bruker SampleTRACK V2.42.18 to:
C:\Program Files\BRUKER\SampleTRACK\

Choose “Install Sampletrack Client System”.

Figure 27.38.The Setup Type Window



Bruker SampleTRACK V2.42.18 - InstallShield Wizard

Setup Type

Choose the setup type that best suits your needs.

Please select a setup type.

○ **Install SampleTRACK System**

All program features will be installed. (Requires the most disk space.)

● **Install SampleTRACK Client System**

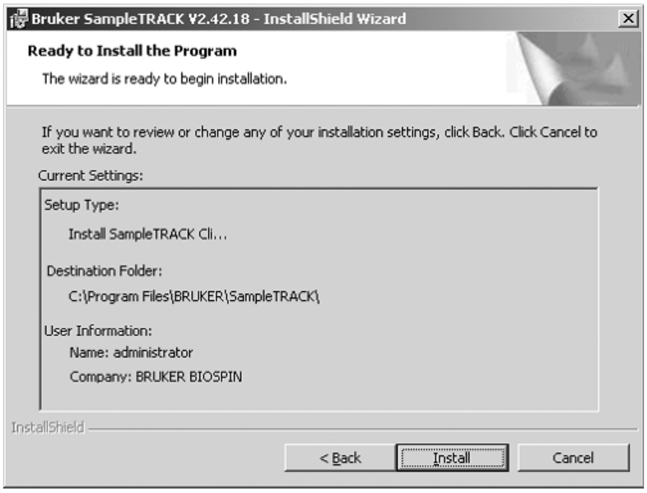
Installs only SampleTRACK Client and Easy Dialog

○ **Customize Features**

Choose which program features you want installed and where they will be installed. Recommended for advanced users.

Press ***Install*** *to start the installation.*

Figure 27.39.The Install Window



Bruker SampleTRACK V2.42.18 - InstallShield Wizard

Ready to Install the Program

The wizard is ready to begin installation.

If you want to review or change any of your installation settings, click Back. Click Cancel to exit the wizard.

Current Settings:

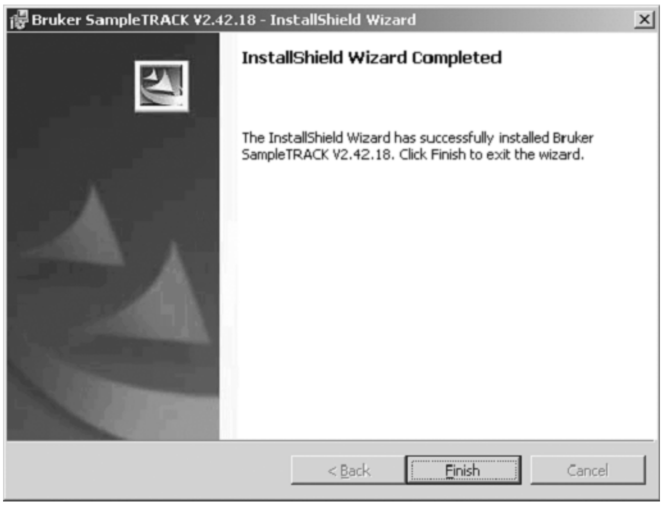
Setup Type:
Install SampleTRACK Cli...

Destination Folder:
C:\Program Files\BRUKER\SampleTRACK\

User Information:
Name: administrator
Company: BRUKER BIOSPIN

SampleTrack client installation is completed.

Figure 27.40.InstallShield Wizard Completed Window



InstallShield Wizard Completed

The InstallShield Wizard has successfully installed Bruker SampleTRACK V2.42.18. Click Finish to exit the wizard.

SampleTrack™ Web Client Installation

28

Introduction / System Requirements 28.1

The SampleTrack Web Client is a web service which offers easy access to the SampleTrack database without installing any client software on the customer's PC. The web service module is only available on

Windows® NT systems

(Windows® 2000, Windows® XP, Windows® 2003)

as a Microsoft® Internet Information Service Module or Apache Module. The Apache Webserver is automatically installed during the installation of SampleTrack. The IIS has to be installed and configured manually.

Depending on the web service usage, the server should be at least a Pentium IV with minimum 512 MB RAM.

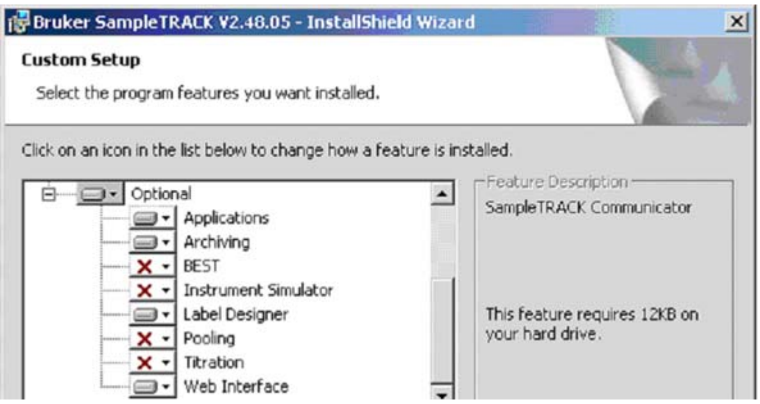
Since the configuration must be done directly on the Web server, the PC should be available directly or via a terminal session.

Installation 28.2

Installation of Program Files 28.2.1

Install the SampleTrack software package on the server, that will be used as a **Web Server** later on. Be sure to select **Customize Features** and activate the item **Web Interface**.

Figure 28.1. InstallShield Wizard Custom Setup



Bruker SampleTRACK V2.48.05 - InstallShield Wizard

Custom Setup

Select the program features you want installed.

Click on an icon in the list below to change how a feature is installed.

- Optional
  - Applications
  - Archiving
  - ✕ BEST
  - ✕ Instrument Simulator
  - Label Designer
  - ✕ Pooling
  - ✕ Titration
  - Web Interface

Feature Description

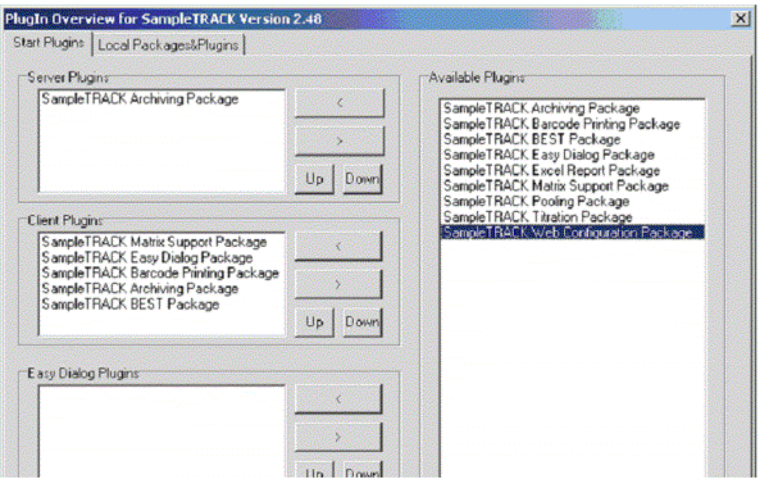
SampleTRACK Communicator

This feature requires 12KB on your hard drive.

Activation of the Web Server 28.2.2

After the SampleTrack installation the Web Interface module is still not activated. Login to the SampleTrack client as administrator. In the menu « Administration » choose „Configure Plug-Ins“.

Figure 28.2. SampleTrack Plug In Overview

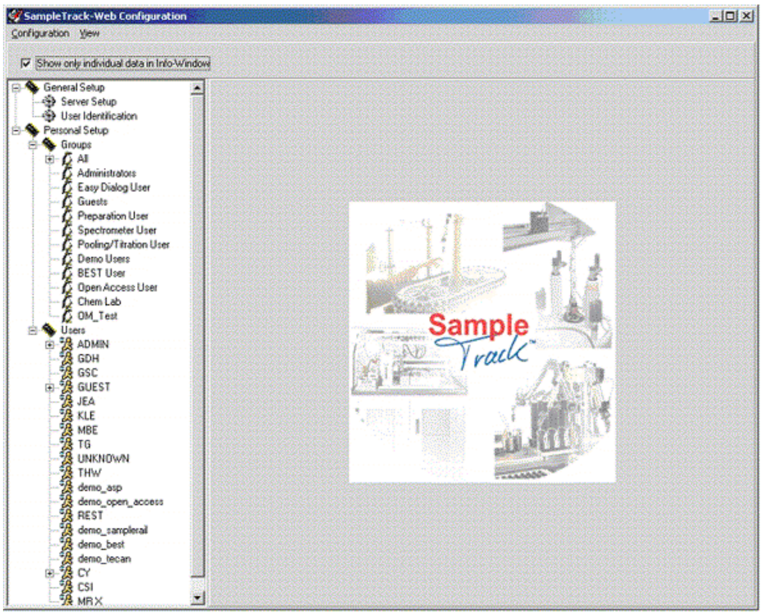

PlugIn Overview for SampleTRACK Version 2.48
Start Plugins
Local Packages&Plugins
Server Plugins
SampleTRACK Archiving Package
<
>
Up
Down
Client Plugins
SampleTRACK Matrix Support Package
SampleTRACK Easy Dialog Package
SampleTRACK Barcode Printing Package
SampleTRACK Archiving Package
SampleTRACK BEST Package
Easy Dialog Plugins
Available Plugins
SampleTRACK Archiving Package
SampleTRACK Barcode Printing Package
SampleTRACK BEST Package
SampleTRACK Easy Dialog Package
SampleTRACK Excel Report Package
SampleTRACK Matrix Support Package
SampleTRACK Pooling Package
SampleTRACK Titration Package
SampleTRACK Web Configuration Package

Select the **Web Configuration Package** and add it to the „Client Plugins“.

Close and restart the SampleTrack client. In the menu “Administration”, select the new option „Configure Web Interface...“.

The new configuration program will be displayed and shows a group tree on the left with different configuration sections. When a configuration section is selected, the current configuration is shown on the right side. Use the button “Change Data” to change the view.

Figure 28.3. Group Tree Window



To install and start the Web Server choose „General Setup“ and „Server Setup“.

In the setup you must start the service as an Apache module or IIS module.

When selecting the IIS module be sure that IIS has been installed correctly before.

Click “Install” to install the service.

From this configuration window you can conveniently start and stop the Web service.

After successful installation a status window displays “Service started”. Clicking on “Browser” opens the browser window with the SampleTrack Web client start page.

Secure Socket Layer (SSL-HTTP) 28.2.3

It is possible to use the SampleTrack Web service with a secure connection (SSL).

This is independent from the SampleTrack configuration and involves the Apache or IIS server configuration. Please contact your IT department for more information.

Configuration 28.3

The SampleTrack Web configuration menu offers more options to customize your automation and individual interface. Apart from the „Custom-Page-Wizard“ each SampleTrack client also provides individual adaption possibilities.

User Identification 28.3.1

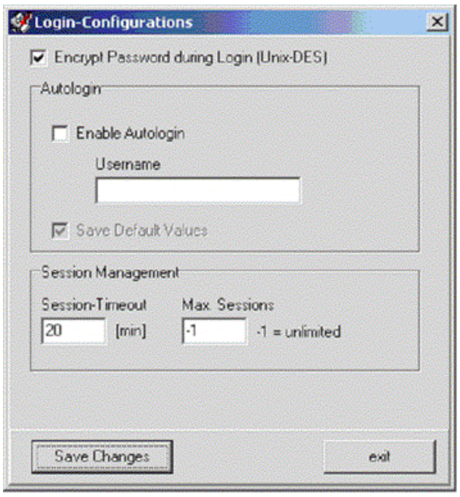
The „User Identification“ and „General Setup“ define the kind of authentification.

With anonymous login (Autologin) a login is not required. To use the Autologin enter the user name which is used for logging into the system.

Session management: Here the session time, length a session should stay open, and the maximun number of concurrent sessions can be defined.

Hint for changing the password: When the SSL is not used, passwords are transferred unencrypted. This is also true, when passwords are being changed, even when „password encryption“ was activated before.

Figure 28.4. Login Configurations



☑ Encrypt Password during Login (Unix-DES)

Autologin

☐ Enable Autologin

Username

☑ Save Default Values

Session Management

Session-Timeout 20 [min]

Max. Sessions -1 -1 = unlimited

Group or Individual User Settings 28.3.2

All further modifications to the HTML pages are group or user specific.

Select the user or group profile from the group tree on the left side. For changes concerning all users select the group “All”.

When a group has no sub-details, this indicates that no specific modifications have been made for the group.

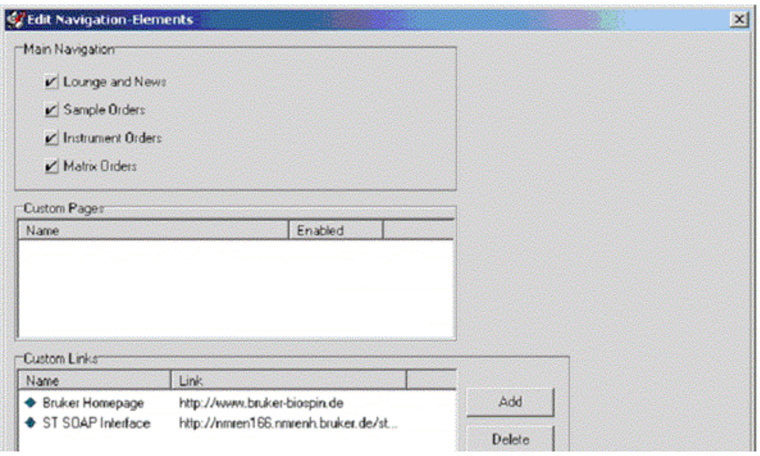
The configuration can be modified with a right click on the group and by selecting **Edit this item**.

Navigation Board

The configuration menu „Navigation“ has options effecting the look and feel of the naviagtion board.

Here you can activate or deactivate the different views, or add additional links, e.g. to your own Intranet homepage. If you do not use a matrix system, you may deactivate this point.

Figure 28.5. Navigation Elements Window



Main Navigation

☑ Lounge and News

☑ Sample Orders

☑ Instrument Orders

☑ Matrix Orders

Custom Pages

Name	Enabled

Custom Links

Name	Link
◆ Bruker Homepage	http://www.bruker-biospin.de
◆ ST SOAP Interface	http://nmren166.nmrenh.bruker.de/st...

Layout

If you have modified the HTML template pages (see the section HTML packages) to adapt them to your corporate design, the layout section allows you to customize the internal design components. You can also define the color to highlight the sample orders.

Custom-page Wizard

The custom page wizard helps you to integrate your own HTML pages and views into the system.

Principally a HTML file is needed. It may have pictures inside. The program is optimized for HTML pages generated with Microsoft® Word ("Save as Web page").

To add a new HTML page enter a page title (it will be displayed within the navigation board) and select the HTML page.

The „Advanced Settings" options define the way the new page should be integrated:

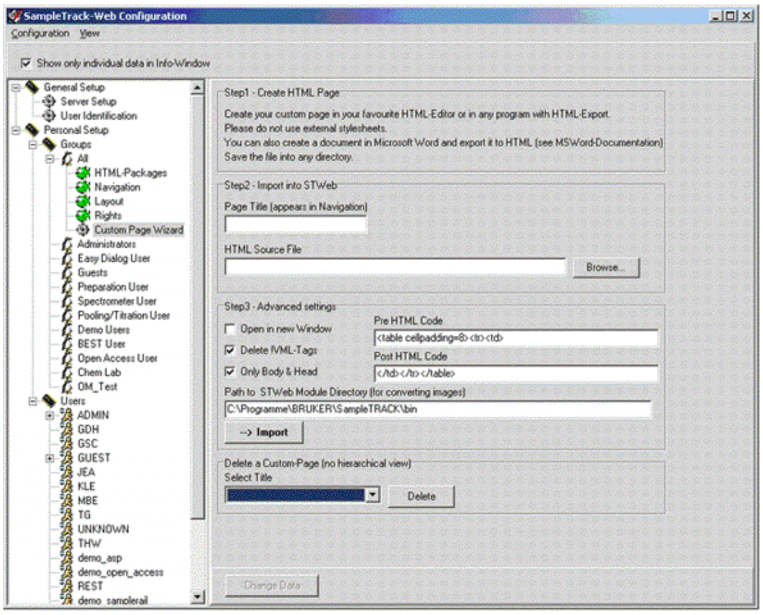
Use **Open in new window** to open the page in a new window without the SampleTrack heading and navigation.

When using more complex HTML pages, it may happen, that the view is not the same as the original design. Try to solve the problems using the checkboxes **Delete VML-Tags** and **Only Body&Head**.

Be certain that SampleTrack Web Module path is set correctly, e.g. when using an Apache server: „C:\Programme\BRUKER\SampleTRACK\web\apache\modules".

Select **Import** to import the HTML page.

Figure 28.6. SampleTrack Web Configuration Window



☑ Show only individual data in Info-Window

Step1 - Create HTML Page

Create your custom page in your favourite HTML-Editor or in any program with HTML-Export.
Please do not use external stylesheets.
You can also create a document in Microsoft Word and export it to HTML (see MSWord-Documentation)
Save the file into any directory.

Step2 - Import into STWeb

Page Title (appears in Navigation)

HTML Source File

Step3 - Advanced settings

☐ Open in new Window
☑ Delete VML-Tags
☑ Only Body & Head

Pre HTML Code: `<table cellpadding=8><tr><td>`

Post HTML Code: `</td></tr></table>`

Path to STWeb Module Directory (for converting images): C:\Programme\BRUKER\SampleTRACK\bin

Delete a Custom-Page (no hierarchical view)

Select Title

HTML Packages

The SampleTrack Web Service are delivered as packages. While the package „Standard“ consists of the necessary basics, more custom specific packages can be added. To import a package select the “.inf” file in the package main directory. Always install the standard package first, and afterwards any additional packages, so they override standard package files.

With a double click on a file you can view and edit the HTML code. After modification of a file the package status changes to “Dev” (development) and the original version is stored, so that a redo of the last modification is always possible.

To uninstall a package, right click on the file name and select „delete package“ from the context menu.

Use the selection „Export Files“ to export the files and edit them with a HTML editor.

Use the selection “Import file” to import new files into the system.

Remember, that a lot of HTML files include control commands for the visualization of database information. This information should not be changed when editing the file.

Rights

When editing the rights for the SampleTrack Web Client you can release EasyWeb Dialogs for a user, activate quick menus / Workstep Tool Boxes, mask and unmask sub menus.

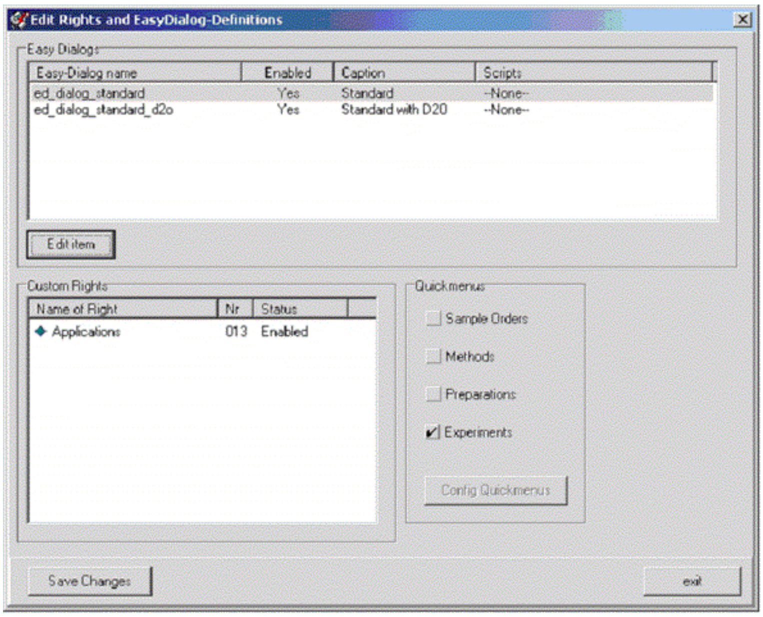
In the Web configuration window all available EasyWeb Dialogs are listed. Select one and click edit.

In the window that appears you can modify the title, the authorization and the executable scripts.

In the window „Custom Rights“ authorization can be changed by checking or uncheck the rights.

At this development level there is only one authorization to activate or deactivate: „Applications“. It allows or forbids access to view experiment results.

Figure 28.7. Edit Rights Window



Edit Rights and EasyDialog-Definitions

Easy Dialogs

Easy-Dialog name	Enabled	Caption	Scripts
ed_dialog_standard	Yes	Standard	--None--
ed_dialog_standard_d2o	Yes	Standard with D20	--None--

Custom Rights

Name of Right	Nr	Status
◆ Applications	013	Enabled

Quickmenus

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