User manual

Toolbox 3.3 Client-Server Configuration
Document history

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If you have questions or comments that relate to this document, please send them to ehscont@oecd.org or visit the QSAR Toolbox discussion forum at https://community.oecd.org/community/toolbox_forum.
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1 Introduction

The Toolbox Server is distributed as a Windows MSI package. It contains the files comprising the Toolbox Server and a Database to be used by the client Toolbox installations. The installation procedure performs only basic COM registration and does not perform any setting up of security permissions/policies needed for the working of the server.

The administrator of the server has the responsibility for configuring the security permissions used for the server’s communication.

2 Prerequisites

2.1 Hardware requirements

The computer hosting Toolbox server must have at least:

- RAM: 2 GB (recommended 4 GB)
- Hard disk space: 12 GB (recommended 20 GB)
- CPU: Dual core processor 2Ghz or greater, 32 or 64 bit architecture (recommended quad-core CPU on 64 bit Operation system)
- Network adapter 100 Mbps (recommended 1Gbps)

2.2 Software requirements

Firebird 2.1 32 bit and 64bit* installation.

* Toolbox uses native client library (fbclient.dll) provided within the firebird installation as the Toolbox server as a 32 bit application is able to load only 32 bit client library to access the firebird server. To be able to use 64 bit server you should provide 32bit version of fbclient.dll.

3 Installation of the Toolbox Server

Please unzip the Toolbox Server installation package on your local disk and run the StartInstall.exe

3.1 Configuration of the Toolbox Server computer

The Toolbox server is a Distributed Component Object Module (DCOM) automation server. In this respect all common rules for the DCOM applications are also valid for the Toolbox server.

3.1.1 Server Firewall settings:

Add Toolbox Server application (TBServerV30.exe) to the exceptions list.
Add TCP port 135 to firewall exceptions list.
3.1.2 Server DCOM configuration:

Authentication policy:

Define a single user on the server machine that all client applications then use to authenticate themselves to the server machine’s operating system. For the purpose of this document this user will be called “ToolboxSvr”.

1. Start DCOMCNFG utility

![DCOMCNFG utility](image)

**Note:** For the 64bit versions of the Windows please use **Start -> Run -> mmc comexp.msc /32** to run DCOM configure utility in 32bit mode.

2. Select properties from the popup menu for “My Computer”.

![My Computer properties](image)

3. Go to the “DCOM config“ item on the left-hand side tree-view, right click on the “ToolboxServerV32“ and select **Properties**.
4. On the **Security** tab select **“Customize”** and click on the **Edit** button for the **“Launch and Activation Permissions”** section. Add **ToolboxSvr** to the list and check **Allow** for “Remote Launch” and “Remote Activation” permissions for the user.

5. On the security tab section select “Customize” and click on the **Edit** button for **Access Permission** section. Add **ToolboxSvr** to the list and check **Allow** for “Remote Activation” permission for the user.
6. From the **Identity** tab select "**The interactive user**". These are the recommended settings. The different **Identity** settings are explained below.

**The interactive user**: server is started in the session of the current user logged onto the system.

- **pros**: Application is started with user interface.
- **cons**: If there is more than one logged user the server is not able to start. The logged user may not have the security rights to activate or access the server.

**The launching user** - not recommended to use

**This user** - server is started in separate session of the specified user

- **pros**: Application always starts.
- **cons**: The user interface is not accessible.

**3.1.3 Server running domain controller DCOM configuration:**

Domain User who will use the server should be added to the “Distributed COM Users” group. The domain is tested on windows 2008R2 Server.
From “Administrative tools” open “Active Directory Users and Computers”.

On the right tab select “Users”

In the left tab select user and click on right mouse button

On appeared context menu select “Add to a group” menu item.
4. Enter “**Distributed COM Users**” in the edit box and then click on “OK” button.

![Select Groups dialog box](image)

5. Repeat steps 3 and 4 for all users which have to access the Toolbox server.

6. Start DCOMCNFG utility Start->RUN ->DCOMCNFG.

**Note:** For the 64 bit versions of the Windows please use **Start -> Run -> mmc comexp.msc /32** to run DCOM configure utility in 32 bit mode.
8. Click Default COM Security.
9. Under Default Access Permissions click Edit Default. Make sure “Distributed COM Users” and provide all have Local and Remote Access permissions.

10. Under Default Access Permissions click Edit Limits. Make sure “Distributed COM Users” and provide all have Local and Remote Access permissions.

11. Under Default Launch Permissions click Edit Default. Make sure Distributed COM User ” and the user whose authentication credentials will be used to access the COM application all have Local and Remote Launch permissions, as well as Local and Remote Activation permissions.

12. Under Default Launch Permissions click Edit Limits. Make sure Distributed COM Users” and the user whose authentication credentials will be used to access the COM
application all have Local and Remote Launch permissions, as well as Local and Remote Activation permissions.

4 Installation of the Toolbox Client

Standalone version of the toolbox can be also used as a Toolbox client.

Please unzip the Toolbox installation package on your local disk and run the StartInstall.exe.

4.1 Configuration of the Toolbox Client computer

4.1.1 Client Firewall settings
Add Toolbox 3.2 application (Toolbox 3.2.exe) to firewall’s exceptions list.

Add TCP port 135 to firewall exceptions list.

4.1.2 Client DCOM configuration:
1. Start the DCOMCNFG utility (Start Menu -> Control Panel -> Administrative tools -> Component Services or invoke "DCOMCNFG" from the Start Menu’s Run menu item)
2. Right click on “My Computer” and select Properties from the popup menu.

3. Go to “COM Security” tab and from the “Access Permission” section use the “Edit Default…” and “Edit Limits…” buttons to change the permissions for security principal “Everyone” and “ANONYMOUS LOGON”.

4. Check “Local Access” as well as “Remote Access” for “Security Limits”.

5. Check “Local Access” as well as “Remote Access” for “Default Security”.
4.2 Configuration of the client application

The Toolbox standalone application can also act as a Toolbox client application.

Configuring this requires the Toolbox to have “Remote connect” set instead of the default “Local connection” in the Toolbox options. When “Remote connect” is selected for the Database the user needs to specify the name or address of machine where the Toolbox Server is installed. After this change Toolbox needs to be restarted.

When Toolbox is started as client application the database importing features are disabled. These functions are delegated to the Toolbox server only.
### Toolbox 3.3 Client-Server Configuration

#### Data matrix
- Title column width: 330
- Cell width: 120
- Description height: 100

#### Chemical browser
- Column count: 5

#### Structural space mode
- 2D (ignore stereo information)
- 3D (preserve stereo information)

#### Database
- **Local Connect**
- **Remote Connect**
- **Server:** localhost
- **Assign Data by SMILES**
- **Use Inventories in chemical input**
- **Pass progress object to server**

#### Folder for user models
- C:/Users/.../Documents/QSAR_Toolbox/QSAR_Toolbox 3.0/UserDir/

#### Calculations
- Do not use parameter cache
- Memory cache size (values or calculator): 5000
- Max count of tautomers for parameter calculation and profiling: 100
- Max SMILES length for 3D calculations: 50

#### Data format
- List separator: 1
- Range separator: ;
- Count of digits: 3

#### Warning messages
- When define chemical group
- When define chemical group with inventories
- When gather data
- When execute query tool
- When profiling with metabolism

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**Toolbox 3.3 Client-Server Configuration**

**Document Version 1.7**

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Connecting to the Toolbox Server

After the client side DCOM is properly set up the Toolbox Client application only needs the IP address (or name) of the Toolbox server.

4.2.1 Non Domain client:
When the Toolbox starts the user is asked to provide credentials for the Toolbox server.

Select “As User” and enter username and password of the account who have defined access to the Toolbox Server application on the remote machine for this presentation is the ToolboxSvr.

4.2.2 Domain Client
On the Toolbox remote wizard leave the selection “As current user” and then click “OK” the current user will be used to log to the server.
4.3 Troubleshooting DCOM

4.3.1 Configuration check list

Common for domain and non domain configurations:

DCOM is enabled on both client and the server

The Toolbox Server is configured to run in “Interactive mode” (it is possible to define it “as user” but the user interface will not be accessible).

The Firewall does not block connections on both client and server.

On the client the firewall is configured to allow the Toolbox application inbound and outbound connections and TCP/IP port 135 is open for outbound connections.

On the server the firewall is configured to allow ToolboxServer application inbound and outbound connections and TCP/IP port 135 is open for outbound connections.

When in Non-Domain configuration:

There is a defined user account (for instance “ToolboxSvr”) on server and client with same name and password.

The Toolbox account (“ToolboxSvr”) is logged into the server.

Toolbox account has privileges in the DCOM configure section to access, launch and activate ToolboxSvr object on both client and the server.

Clients connecting to the server provide user name and password.
When in Domain configuration:

All domain users have granted DCOM access, launch and activation rights.
The server object runs under an account granted with access, launch and activate rights.
Clients access the server from Toolbox start-up screen as “current user”.

### 4.3.2 Common errors

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<th>Possible Issues</th>
<th>Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>The RPC server unavailable</td>
<td>The computer really doesn't exist.</td>
<td>Add Toolbox server application(TBServerV3.exe) to the firewall’s exceptions list and open TCP/IP port 135.</td>
</tr>
<tr>
<td></td>
<td>The Windows Firewall on the server is blocking the connection.</td>
<td></td>
</tr>
<tr>
<td>Access denied</td>
<td>DCOM is not enabled.</td>
<td>1. Check if server and client firewalls allow connections.</td>
</tr>
<tr>
<td></td>
<td>Client firewall blocks connection.</td>
<td>2. Check if server runs under account that has DCOM rights.</td>
</tr>
<tr>
<td></td>
<td>The user does not have remote access to the computer through DCOM.</td>
<td></td>
</tr>
<tr>
<td>Client is compiled with different server access library...</td>
<td>The client and server versions does not match.</td>
<td>Update Toolbox server and Toolbox Client to the latest version.</td>
</tr>
</tbody>
</table>
### Interface not supported

The implementation Toolbox Server interface of the server differs from the client implementation or the client.

Update Toolbox server and Toolbox Client to the latest version.

### Unable to bind client ITBNotify callback interface to the server

Client does not allow callbacks from the server. The server runs under user account with no defined granted DCOM rights on the client.

Grant access, launch and activate permissions to the server’s user account on the client.

### The server process could not be started because the configured identity is incorrect. Check the User name and Password.

There is no logged user on the server or the logged user does not have granted DCOM rights on the Toolbox Server.

**Option 1 :**

Change the settings of the Toolbox server object from DCOMCNFG to work “as user” from the identity.

**Option 2:** Grant DCOM access, launch and activate to the current user logged the system.