

Volume

1

IDEACONSULT

Toxmatch Installation Manual

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Introduction

Toxmatch is a fully-featured and flexible user-friendly open source application, which encodes a variety of chemical similarity indices including several structural and descriptor based chemical similarity indices. A number of file formats are supported.

The Toxmatch application is suitable for use on a standalone PC. It has been designed with flexible capabilities for future extensions (e.g. other similarity schemes that might be developed in the future).

Prerequisites

Toxmatch requires Java™ 2 Runtime Environment, Standard Edition 1.5 or newer on the target system and it is platform-independent. It runs under any host operating system, which supports Java™ 2 Runtime Environment, Standard Edition.

The hardware requirements include 256 MB free disk space and a minimum of 256 MB available RAM (512 MB or more is highly recommended).

Toxmatch distributions

Toxmatch is distributed in two different ways:

- ZIP archive, containing the complete documented Java™ source code, binaries, training data sets for four predefined toxicity endpoints (*Aquatic toxicity*, *Bioconcentration factor*, *Skin sensitization* and *Skin irritation*), installation manual and user manual;
- Windows™ (NT, 2000, XP or 2003) standalone (offline) automated installer with integrated Java™ 2 Runtime Environment, Standard Edition 1.5 setup.

The ZIP archive is suitable for use on any operating system with Java™ 2 Runtime Environment, Standard Edition 1.5 already installed. It might be useful also for studying the application source code.

The Windows™ installer includes all the contents of the ZIP archive, as well as the ability to check for the presence of Java™ 2 Runtime Environment, Standard Edition

1.5 on the target system. If the installer does not detect Java™ 2 Runtime Environment, Standard Edition 1.5 already installed on the target system, it would attempt to install it, prior to proceeding with Toxmatch setup.

Windows™ Toxmatch setup

The Toxmatch application is distributed with fully automated online installer (**Toxmatch-vX.YZ-setup.exe**), compatible with recent versions of the Microsoft Windows (NT, 2000, XP, 2003) operating system. In order to install Toxmatch just run the installer and follow its instructions. It contains all the required packages, including the Java™ 2 Runtime Environment, Standard Edition 1.5 setup. The installer will check the size of available free disk space on your system and will allow you to install Toxmatch only if the above mentioned requirement is met.

If the installer does not detect Java™ 2 Runtime Environment, Standard Edition 1.5 or newer on the target system, it will attempt to install it before proceeding with the Toxmatch setup. In this case, the user running the installer **SHOULD HAVE ADMINISTRATIVE PRIVILEGES** on the target system (otherwise the Java™ 2 Runtime Environment, Standard Edition setup would be aborted and Toxmatch would not be installed).

If the installer detects Java™ 2 Runtime Environment, Standard Edition 1.5 or newer already installed on the target system, it will proceed directly with the Toxmatch setup. In this case, **ADMINISTRATIVE PRIVILEGES ARE RECOMMENDED BUT NOT NECESSARILY REQUIRED.**

When the installer is launched by a user with administrative privileges, it will create Toxmatch start menu shortcuts for all the users registered in the target system. Otherwise, start menu shortcuts will be created only for the unprivileged user, who launched the installation.

After a successful installation, Toxmatch could be launched from the Start Menu (“Start → All Programs → Ideaconsult → Toxmatch-vX.YZ → Toxmatch-vX.YZ”).

Toxmatch setup for other OS

Toxmatch runs under any host operating system, which supports Java™ 2 Runtime Environment, Standard Edition (e.g. Linux, FreeBSD, Solaris, Mac OS, etc...). If you're running such operating system, you should download and use the ZIP archive distribution of Toxmatch.

Please, note that before attempting to run Toxmatch, you should check that Java™ 2 Runtime Environment, Standard Edition 1.5 (or newer) is installed on your system. If Java™ 2 Runtime Environment, Standard Edition is missing (or an older version is present), please obtain (from <http://java.sun.com>) and run the appropriate Java™ 2 Runtime Environment, Standard Edition installer for your system.

On all platforms (having Java™ 2 Runtime, Standard Edition 1.5 or newer installed), Toxmatch can be launched by executing the following command (after decompressing the ZIP archive distribution of Toxmatch):

```
java -jar Toxmatch.jar
```

Please, note that in the above mentioned command “java” and “Toxmatch.jar” should be eventually prefixed with the full path to java and Toxmatch on the destination platform.

Uninstalling Toxmatch

Each version of Toxmatch could be uninstalled from Windows™ either by using the “Control Panel → Add or Remove Programs” or by clicking the “Uninstall” link located in “Start → All Programs → Ideaconult → Toxmatch-vX.YZ → Uninstall-Toxmatch-vX.YZ”. Any application files which may happen to be locked during the uninstall procedure would be deleted after the next reboot of the system.

Please, note that Java™ 2 Runtime Environment, Standard Edition would not be uninstalled from Windows™ by the Toxmatch uninstaller. If needed, it could be uninstalled via its own entry in “Control Panel → Add or Remove Programs”.

Users of other operating systems, who want to uninstall Toxmatch, could safely remove the files and folders, which were created by extracting the ZIP archive distribution of Toxmatch.