Toxtree Installation Manual
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# Table of Contents

*Introduction* ................................................................. 1  
*Prerequisites* .............................................................. 3  
*Toxtree distributions* .................................................... 3  
*Windows\textsuperscript{TM} Toxtree setup* ................................ 4  
*Toxtree setup for other OS* ............................................... 4  
*Uninstalling Toxtree* ...................................................... 5
Introduction

Toxtree is a full-featured and flexible user-friendly open source application, which is able to estimate toxic hazard by applying a decision tree approach. Currently it includes the following plug-ins:


- A decision tree for estimating eye irritation and corrosion potential, based on rules published in “Assessment of the eye irritating properties of chemicals by applying alternatives to the Draize rabbit eye test: the use of QSARs and in vitro tests for the classification of eye irritation, Ingrid Gerner, Manfred Liebsch & Horst Spielmann, Alternatives to Laboratory Animals, 2005, 33, pp. 215-237”;


- START (Structural Alerts for Reactivity in Toxtree) biodegradation and persistence plug-in is based on a compilation of structural alerts for environmental persistence and biodegradability. These structural alerts are molecular functional groups or substructures that are known to be linked to the environmental persistence or biodegradability of chemicals. The rulebase utilizes the structural alerts in logical decision trees. If one or more the structural alerts embedded in the molecular structure of the chemical are

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recognized, the system flags the potential persistence or biodegradability of the chemical. Installation and user manuals available²;


- Cramer rules with extensions: This plug-in is a copy of the original plug-in, plus minor extensions. Like the Cramer plug-in, this plug-in works by assigning compounds to Class I, II, or III, according to the rules from Cramer, and some extra ones. Several compounds were classified by Munro in 1996⁴ as Class I or Class II compounds according to the Cramer rules, even though Munro reported low NOEL values upon oral administration (indicating relatively high toxicity). To overcome such misclassifications, five rules have been introduced to capture the possible toxicity of these compounds;


- Skin sensitization alerts, as per Enoch SJ, Madden JC, Cronin MT, Identification of mechanisms of toxic action for skin sensitisation using a SMARTS pattern based approach, SAR QSAR Environ Res. 2008; 19(5-6):555-78;


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concern (TTC): guidance for application to substances present at low levels in the diet. Food Chem. Toxicol. 42, 65–83;


Toxtree could be applied to datasets from various compatible file types. User-defined molecular structures are also supported - they could be entered by SMILES, or by using the built-in 2D structure diagram editor.

The Toxtree application is suitable for a standalone PC. It has been designed with flexible capabilities for future extensions in mind (e.g. other classification schemes that could be developed at a future date). New decision trees with arbitrary rules can be built with the help of graphical user interface or by developing new plug-ins.

Prerequisites

Toxtree requires Java™ 2 Runtime Environment, Standard Edition 1.6 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.

Toxtree distributions

Toxtree is distributed in two different ways:

- ZIP archive, containing the complete documented Java™ source code, binaries, example lists of compounds, installation manual and user manual;

- Windows™ (NT, 2000, XP or 2003) standalone (offline) automated installer with integrated Java™ 2 Runtime Environment, Standard Edition 1.6 setup;

The ZIP archive is suitable for use on any operating system with Java™ 2 Runtime Environment, Standard Edition 1.6 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 1.6 on the target system. If the installer does not detect Java™ 2 Runtime Environment, Standard Edition 1.6 already installed on the target system, it would attempt to install it, prior to Toxtree setup.

**Windows™ Toxtree setup**

The Toxtree application is distributed with a fully automated offline installer (Toxtree-vX.Y.Z-setup.exe), compatible with recent versions of the Microsoft Windows (NT, 2000, XP, 2003) operating system. In order to install Toxtree just run the installer and follow its instructions. The installer contains all the required packages, including the Java™ 2 Runtime Environment, Standard Edition 1.6 setup.

If the installer does not detect Java™ 2 Runtime Environment, Standard Edition 1.6 or newer on the target system, it will attempt to install it before proceeding with the Toxtree 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 1.6 setup would be aborted and Toxtree would not be installed).

If the installer detects Java™ 2 Runtime Environment, Standard Edition 1.6 or newer already installed on the target system, it will proceed directly with the Toxtree 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 Toxtree 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, Toxtree could be launched from the Start Menu ("Start►All Programs►Ideaconsult►Toxtree-vX.Y.Z►Toxtree-vX.Y.Z").

**Toxtree setup for other OS**

Toxtree 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 Toxtree.
Please, note that before attempting to run Toxtree, you should check that Java™ 2 Runtime Environment, Standard Edition 1.6 (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.

Uninstalling Toxtree

Each version of Toxtree 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►Ideaconsult►Toxtree-vX.Y.Z►Uninstall-Toxtree-vX.Y.Z". 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 Toxtree un installer. 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 Toxtree, could safely remove the files and folders, which were created by extracting the ZIP archive distribution of Toxtree.