

TerraTox™ Databases

User Manual, vs. 3.1

Copyright © 2006, TerraBase Inc.

Software Purpose

TerraTox™ is a specialized database software, designed and optimized solely for the quick retrieval of available toxicological and physico-chemical data for chemical substances. TerraTox database modules contain between 1,000 and 100,000 individual chemical substances each. The available information for each substance varies, but up to ~250 different types of data are available for the more common compounds. References are shown for the more significant properties. Chemical structures are shown in 2D or 3D (user determined).

The TerraTox software has the most powerful search routines available in the industry, allowing simultaneous search by chemical structure, name, formula, CAS, and any two of the up to ~250 types of effects listed in the specialized TerraTox databases. This search ability results in unparalleled speed, convenience, and success in finding the information sought.

TerraTox™ Database Modules

At this time, the following TerraTox modules are available. For details on the databases below, please see the [TerraBase](#) web site, or use the hyperlinks below.

TerraTox™ - [Drugs](#)
TerraTox™ - [Explorer](#)
TerraTox™ - [HIV-1](#)
TerraTox™ - [Pesticides](#)
TerraTox™ - [Tetrahymena](#)
TerraTox™ - [Skin](#)
TerraTox™ - [Steroids-RBA](#)
TerraTox™ - [Vibrio fischeri](#)

New and expanded modules will come on stream from time to time. Please check our web site or send an email message with a request to be informed on specific developments.

TerraQSAR™ Computation Modules

Our valued customers are also advised on the concurrent development of our TerraQSAR™ computation programs. For details, please see the [TerraBase](#) web site.

Table of Contents

Software Purpose	1
TerraTox™ Database Modules	1
TerraQSAR™ Computation Modules.....	1
Table of Contents	2
List of Figures	2
List of Tables	2
Introduction.....	3
Opening Window	3
Module Select	4
Searching.....	4
Name Search	5
Formula Search	7
CAS Search.....	8
Structure Search.....	9
Property Search.....	11
Simultaneous Search of Two or More Fields	13
3D Viewer.....	13
Note regarding 3D structures	15
SMILES Notation	16
Literature.....	16
Acknowledgement	17
Security Features.....	17
Legal	18
License Agreement	18
Trademarks and Copyrights	22
Technical Requirements.....	22
Installation Instructions.....	23
Customer Support	23

List of Figures

Figure 1. TerraTox opening window.....	3
Figure 2. Module Selection box.	4
Figure 3. Search window overview.	5
Figure 4. Standard Name search.....	6
Figure 5. Advanced Name search.....	7
Figure 6. Formula Search window.	8
Figure 7. CAS Search window	9
Figure 8. Chemical structure search window.	10
Figure 9. Chemical structure search window with SMILES string.....	11
Figure 10. Property search window.....	12
Figure 11. Property search result.....	12
Figure 12. Search status window.....	13
Figure 13. Detailed compound information and 2D structure.....	14
Figure 14. Detailed compound information and 3D structure (a).	14
Figure 15. Detailed compound information and 3D structure (b).	14
Figure 16. 3D Viewer display.	15

List of Tables

Table 1. Valid and invalid examples of Accelrys' SMILES code.....	16
---	----

Introduction

Welcome to the **TerraTox™** databases, a series of unique database software modules, which can simultaneously be searched by name, chemical formula, CAS number, chemical structure, or fragments thereof, and up to two concurrent field values (numerical or text). **TerraTox™** databases have been developed by [TerraBase Inc.](#)

TerraTox database products are designed for easy use and provide the most important information for chemicals from the relevant scientific literature. They are maintained and updated regularly by reference to the most recent publications.

TerraTox database products are valuable research tools in the fields of health, environment, pharmaceuticals, and general chemistry.

Opening Window

The TerraTox module will display the initial TerraBase Inc. logo and its address, the user name and affiliation, the copyright and related information. This screen is normally visible for a few seconds only upon accessing the software, but can also be accessed anytime from the **Help/About** menu item, as shown on Fig. 1. Location of [Module Select](#), [Search](#), and [View](#) functions are shown, as well as the Help/About command location.

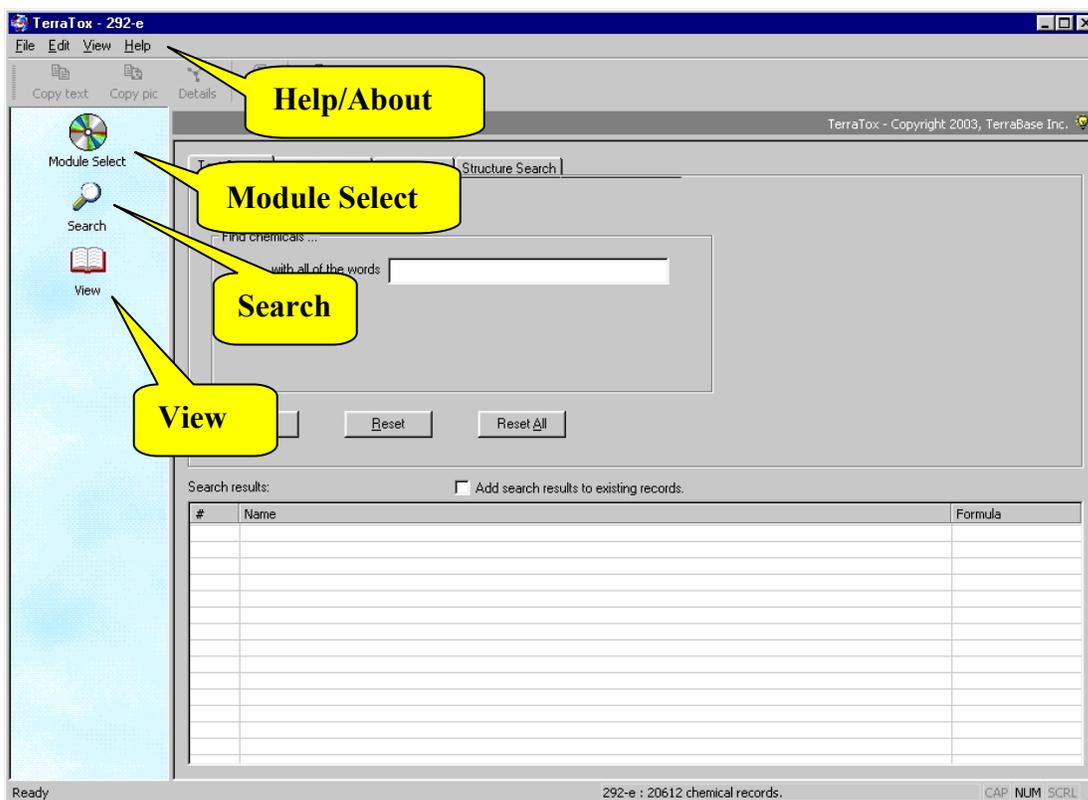


Figure 1. TerraTox opening window.

Module Select

For users subscribing to two or more databases, upon clicking on the Module Select icon, a list of available choices will appear, as shown in Fig. 2, the list of modules available depends on the user's subscription choices. The main field shows currently available modules.



Figure 2. Module Selection box.

Searching

The TerraTox programs have a variety of search functions built-in. They include (main functions only): [Name](#) search, chemical [Formula](#) search, [CAS](#) number search, chemical [Structure](#) search, and [Property](#) search. The opening screen of the Search window is shown in Fig. 3, showing the main four search capabilities of TerraTox databases.

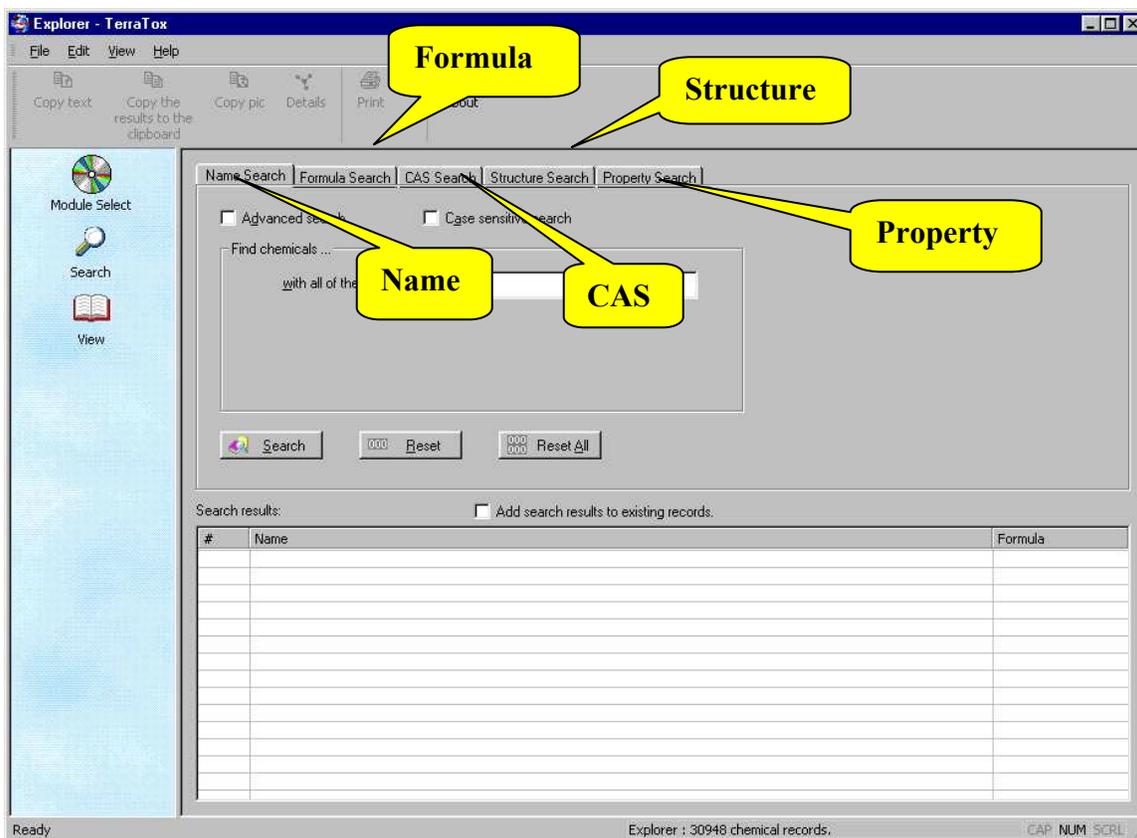


Figure 3. Search window overview.

Name Search

Standard Search

The Name search (standard) allows the user to enter up to seven words or word fragments to search the database of choice for all occurrences which contain all of the given word fragments in the chemicals' name. For example, a search for “phen amin chlor” of the TerraTox – Explorer database results in the listing of compounds as shown in Fig. 4. Please note that the **Name search is not case-sensitive**.

Tip: The order of text fragments in the search field does not affect the search results.

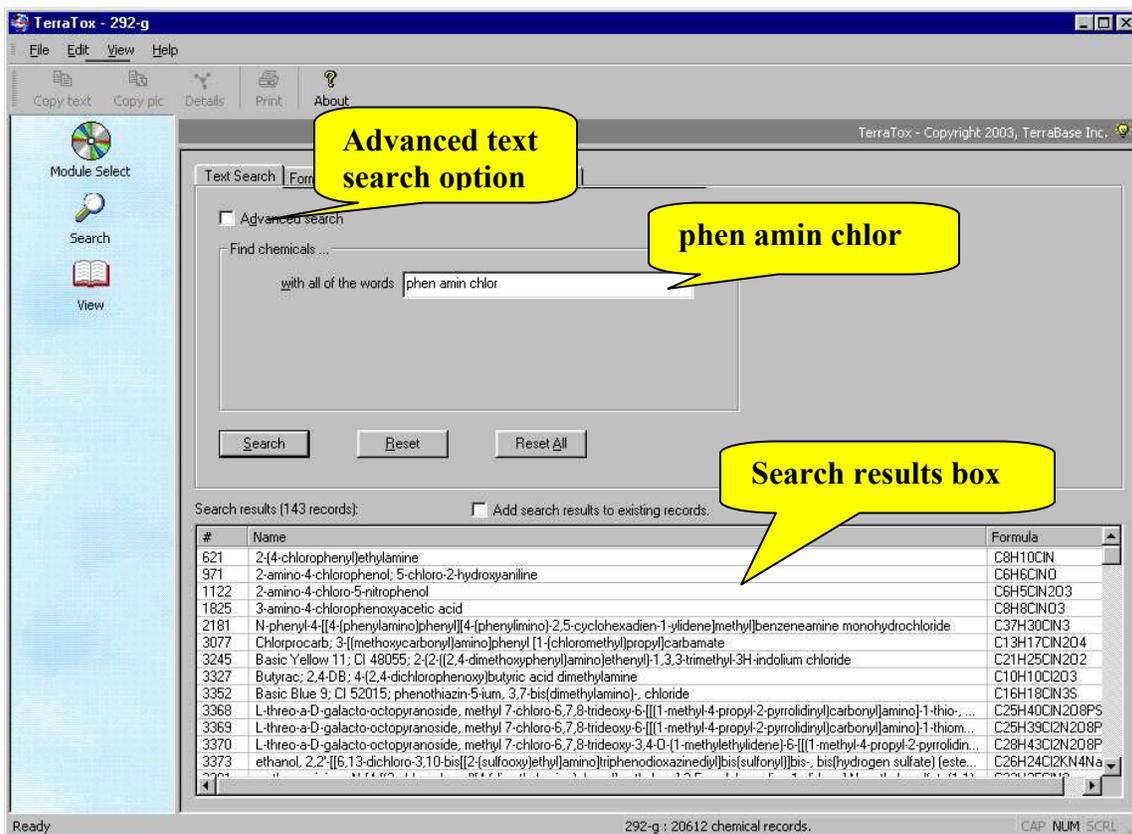


Figure 4. Standard Name search.

Advanced Search

The Name search function has an option for an advanced search, as also shown in Fig. 4. Clicking on the Advanced Text Search option will open the Advanced Text Search window, as shown in Fig. 5. The Advanced Text Search enables to search simultaneously for compounds WITH ALL of the text fragments, WITH AT LEAST ONE of the fragments, and WITHOUT certain fragments. For example, as shown in Fig. 5, a search for compounds WITH the word fragments “phen amin chlor” and WITHOUT the fragment “nitro” in the name results in the list of compounds shown in the results window. Only the first 13 of 135 compounds in the TerraTox – Explorer database resulting from above search are visible in the field. The rest becomes visible upon scrolling down the right hand scroll bar.

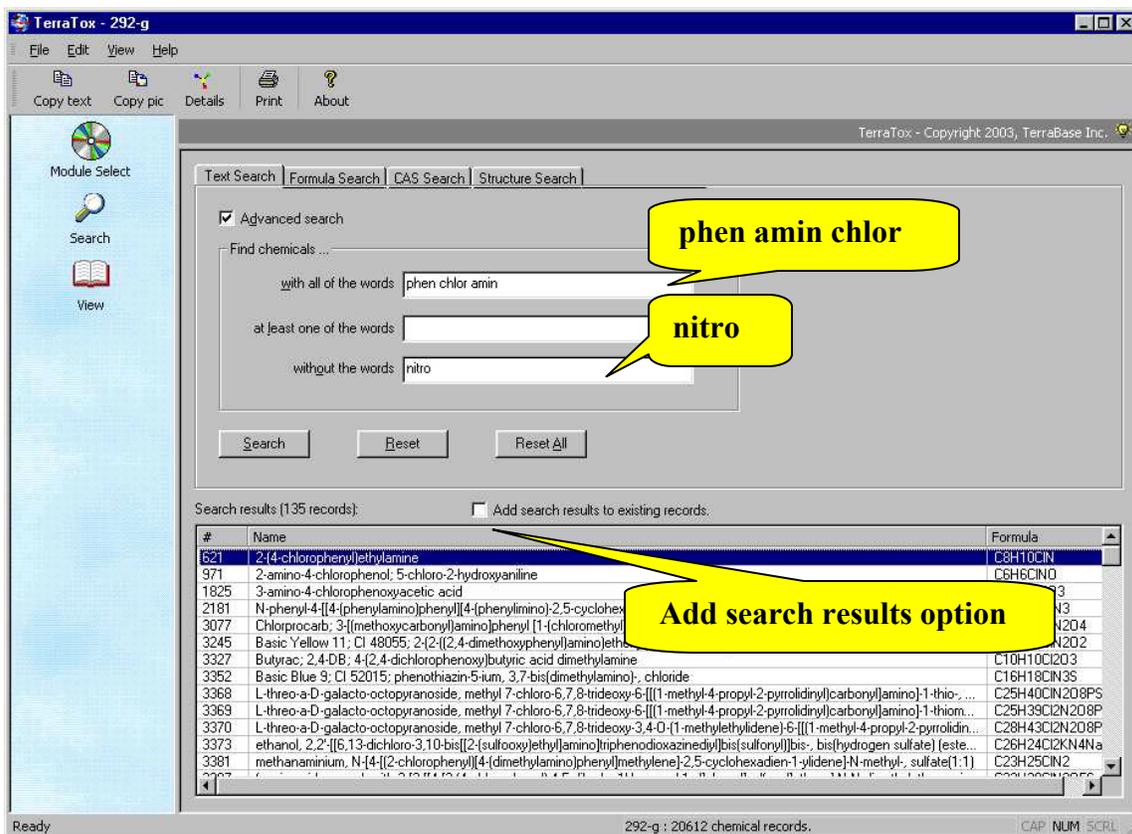


Figure 5. Advanced Name search.

A further Name search option is available, i.e. to search for several terms, such as “phen amin chlor”, but rather than requiring all terms to be in each compound, to have AT LEAST ONE of the search terms in the name. For this option, just place the search term in the middle box of the three Advanced Text Search fields. Search terms can be changed, terms can be added or deleted at will and a new search can be performed with combinations of any of these search conditions. In addition, the results of one search can be saved and the results of the next search can be appended to the list by activating the “Add search results” option, also shown in Fig. 5.

Tip: The order of text fragments in the WITH, AT LEAST ONE, or WITHOUT fields does not affect the search results.

Formula Search

Searching by chemical formula is simple and straightforward. As shown in Fig. 6, formula search can be performed for either a formula fragment (sub formula search option) or for an exact chemical formula (exact formula option). Please note that the **Formula Search is case sensitive**. For example, searching for “r” will result in a list of all compounds with Br, Cr, Sr, Zr, etc. in the chemical formula. In contrast, search for the letter “R” will result in compounds containing Rb, Rh, Ru, etc. When searching for several

atoms simultaneously, such “Br” and Cl” in the same compound, Hill’s rule must be followed and the number of atoms must be specified (except for “1”). For example, searching for compounds with one bromine atom and two chlorine atoms in the molecule must be entered as “BrCl2”.

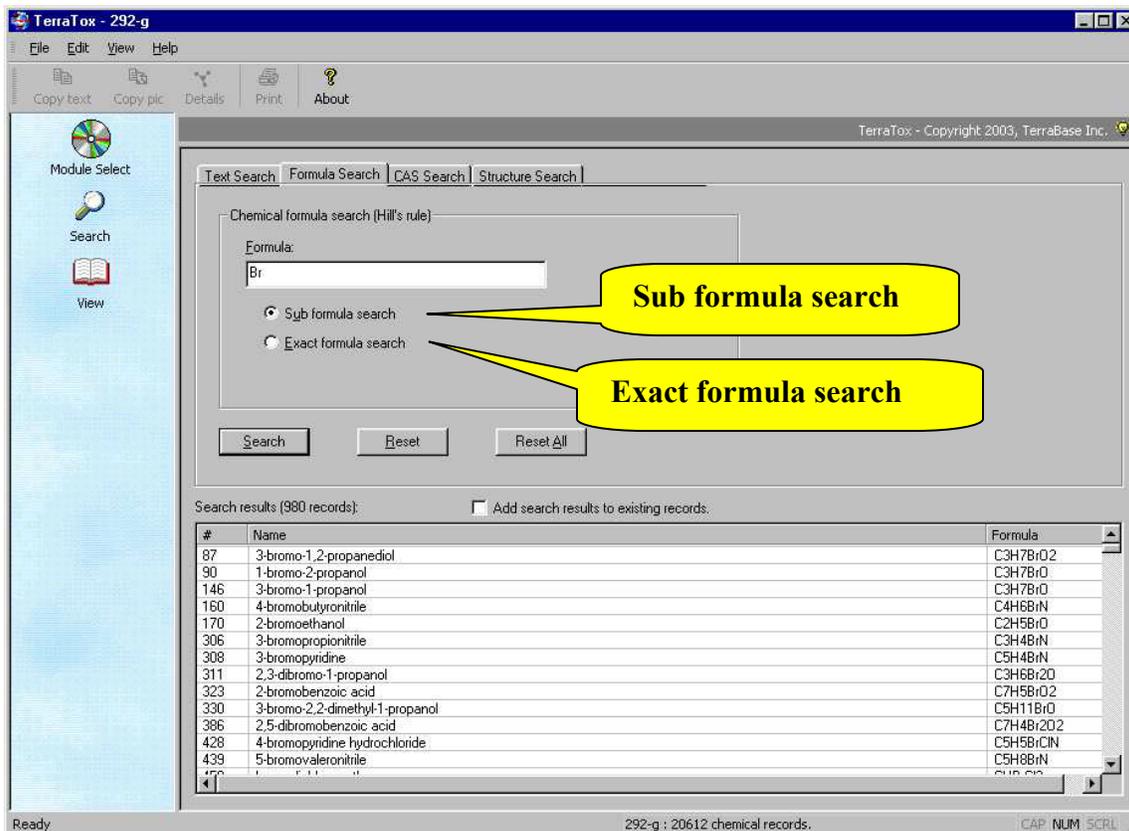


Figure 6. Formula Search window.

Tip: When searching for compounds with several specific types of atoms present, such as bromine, chlorine, iodine, the best method would be to place one of these terms in the Formula search box (e.g. “Br”) and the other ones into the text search box, e.g. “chlor iod” and perform simultaneously both Text and Formula fields.

CAS Search

Chemical Abstracts Service (CAS) numbers for chemicals have the formats shown in the CAS Search window (Fig. 7). It allows to search for compounds with known, or partially known CAS numbers. First, select the appropriate mask (21-11-1, 311-11-1, etc.), and then fill in the available information, or use question marks for missing information. For example, a search for “111-??-?” would find all compounds in the database with CAS numbers starting with “111-“. The maximum number of question marks for unknown digits is nine, i.e. “?????-??-?”. It will find all compounds with CAS numbers 100000-00-? and higher in the specified database.

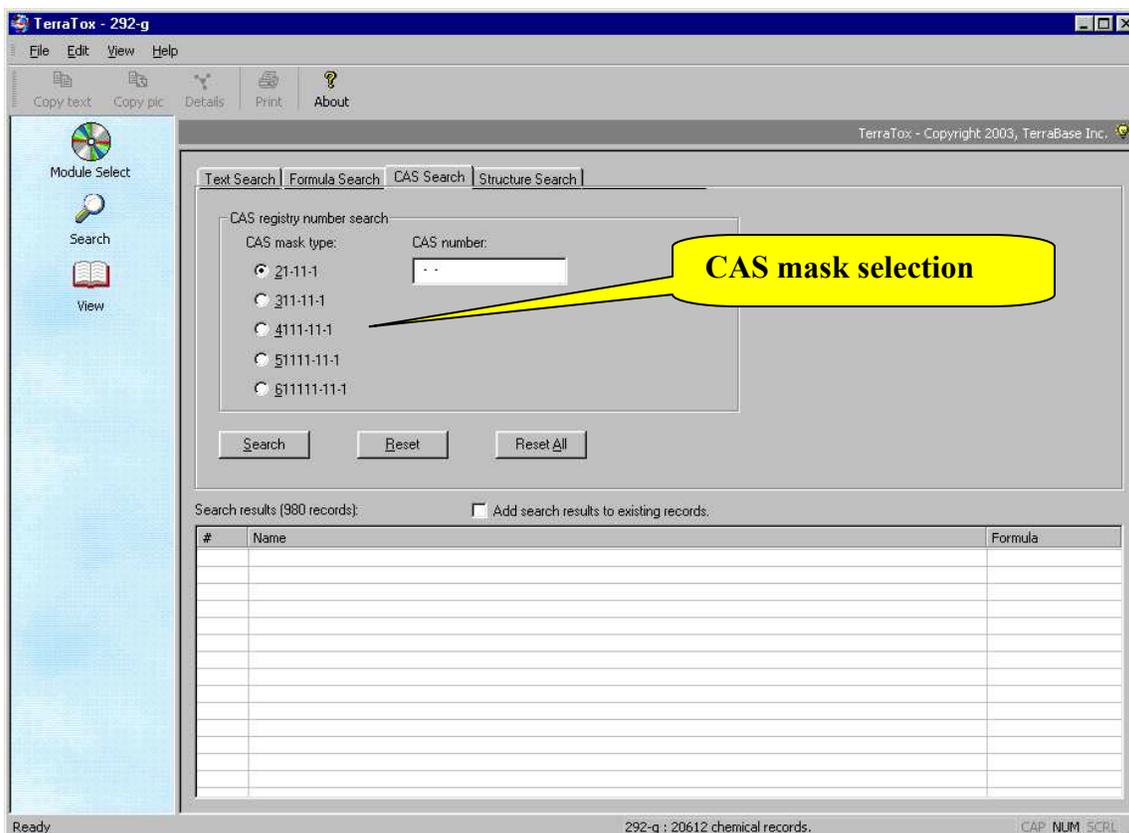


Figure 7. CAS Search window.

Structure Search

TerraTox modules use as chemical structure input a chemical's SMILES code (2D or 3D), which is an international code for the representation of chemical structures and amenable to computer analysis. Numerous chemical structure editors are available freely on the internet and can be used to create or transfer molecular structures into SMILES code, including the built-in [3D-Viewer](#).

The search window for chemical structure fragments is shown in Fig. 8. The chemical structure search window has four search options, namely FRAGMENT (present), EXACT STRUCTURE, FRAGMENT (absent), and SIMILARITY (Tanimoto similarity function, selectable from 0% to 100% similarity). In contrast to the text search, only one of these four structure search types can be executed at any time; however, the chemical structure search can be combined with an un-restricted number of the other search functions, including advanced text, formula and CAS searches, which results in extremely powerful and fast searches of the TerraTox databases.

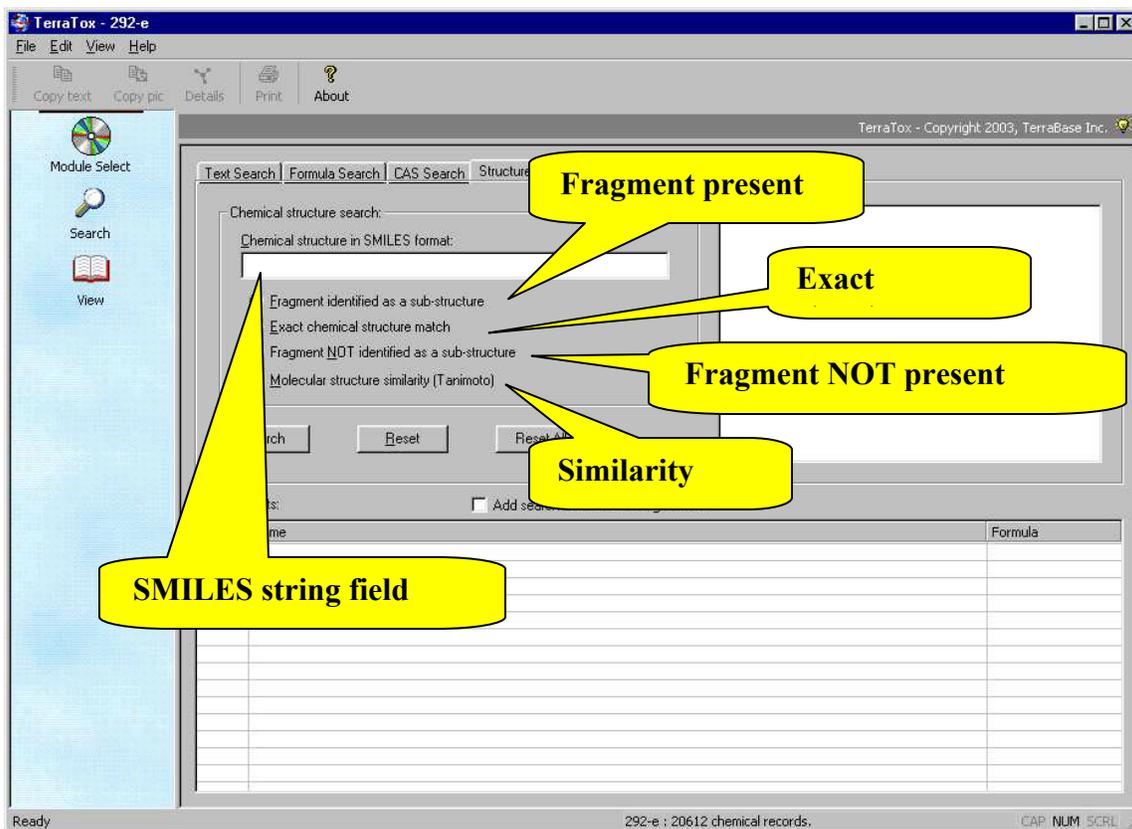


Figure 8. Chemical structure search window.

Whenever a valid SMILES string is entered into the SMILES string field, a chemical graph will automatically appear in the window to the right. This is shown on the example of n-butylbenzene, with the SMILES string “c1ccccc1CCCC” in Fig. 9. For using the 3D display, please refer to the “**3D Viewer**” section, further down.

While only one of the structure search types can be executed at a time, the Accelrys software allows simultaneous search for different atoms in any position, when placed into square brackets. For example, a search for Nc1c([Br,Cl])cccc1 will find all aniline derivatives with either ortho-bromine or ortho-chlorine substituents. There is no limit as to the number of different atoms in the square brackets. For example, a search for Nc1c([Br,Cl,I,F,N,O,S,Se])cc(O)cc1 will find all 4-hydroxy-aniline derivatives with a chlorine, bromine, iodine, fluorine, nitrogen, oxygen, sulfur, or selenium atom in ortho-position to the aniline-nitrogen atom. These substitution rules also apply to cyclic fragments, but observe the rules for aromaticity. For example, a search for n1c[c,n]c[c,n]c1 will find all pyridine, pyrimidine and 1,3,5-triazine derivatives in the database.

Tip: Due to the relatively slower chemical structure search (approximately ~10000 compounds / minute), searching by structure fragment only can be time-consuming when checking larger databases, such as the TerraTox - Explorer database. It is therefore recommended, wherever possible, to combine the structure search with one or more of the other search options. In general, this will greatly increase the speed of the search.

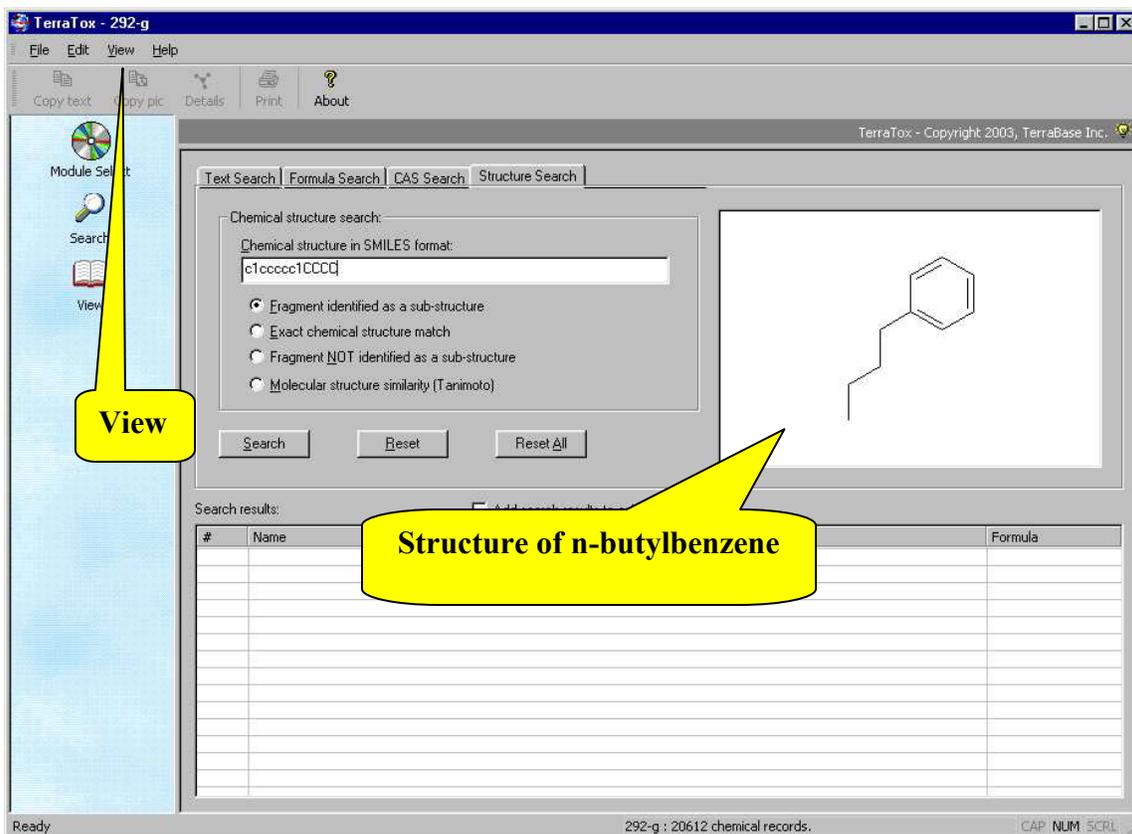


Figure 9. Chemical structure search window with SMILES string.

Property Search

The TerraTox search system also allows for the search of (numeric) **values and text conditions in any of the data fields**. Each TerraTox database has its own list of effect and property fields, which are seen in “**First property**” and “**Second property**” scrollable windows. The following examples are from the Explorer database. On activating the “Property” search tab, as shown in Fig. 3, the Property Search window will appear, as shown in Fig. 10.

The (identical) lists of searchable properties can be scrolled and one parameter field can be selected from each list. As the lists contain both fields with numeric values (such as toxicity values in “pT” notation) and text fields (such as the “**Use / effect**” field), the search options available will change accordingly. For example, clicking on a text-only search term, such as the “Use / effect” line in the “**First property**” window, will result in the “Value search text/number” window to become active together with the “Case sensitive” window.

When clicking on a numeric-value-only search term, such as “**FHM-96 pT**” [fathead minnow 96-hr LC50 in log(L/mmol) units], the “Value search text/number” will become active together with the “**Condition**” window. The (numeric) condition available are (i) equal to (“=”), (ii) greater than or equal to (“>=”), and (iii) lesser than or equal to (“<=”).

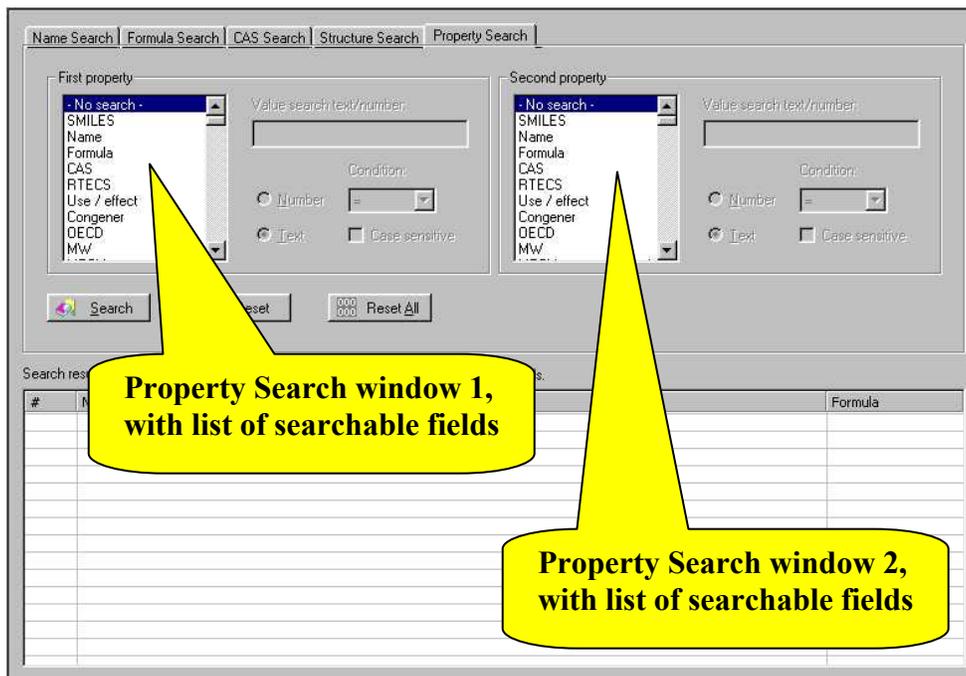


Figure 10. Property search window.

An example of a single numeric property search is shown in Fig. 11. Searching for values with “FHM-96 pT” for a value of “-5” and the condition “>=” will result in a list of more than 900 compounds, as shown in Figure 11.

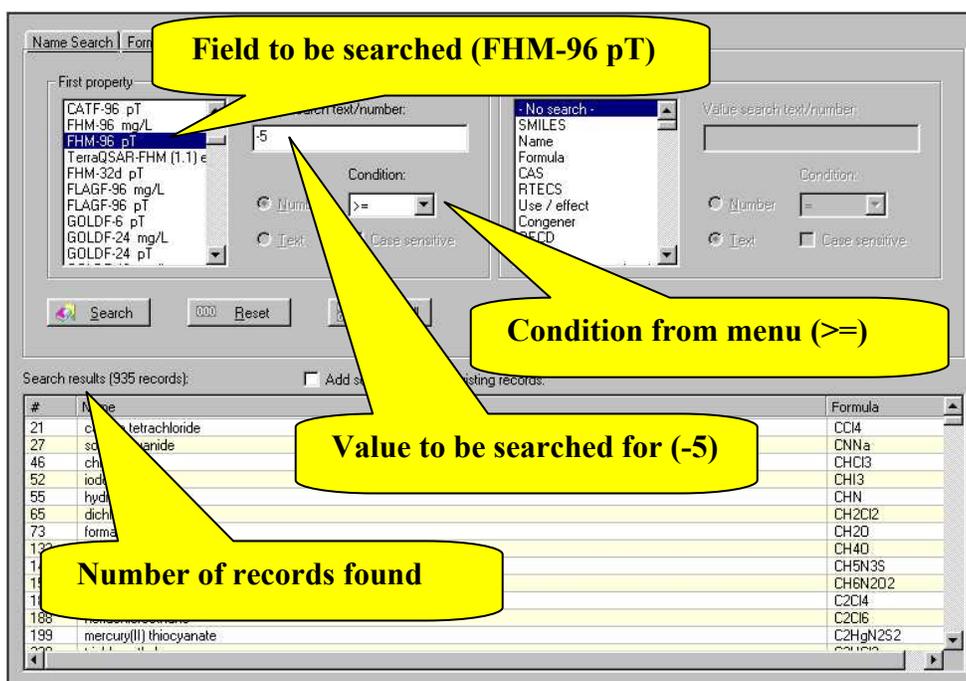


Figure 11. Property search result.

Simultaneous Search of Two or More Fields

As mentioned already, TerraTox databases employ highly sophisticated search systems that allow the simultaneous searching by several search types, namely, name, formula, CAS, structure, and property search. All what is required is entering the desired search parameters into the various fields and a click on the “Search” button.

When performing any search, the **search status window** will appear and inform the user about the type(s) of search which is (are) under way, the search progress, approximate time remaining, and the total number of compounds identified so far. An example is shown in Fig. 12.

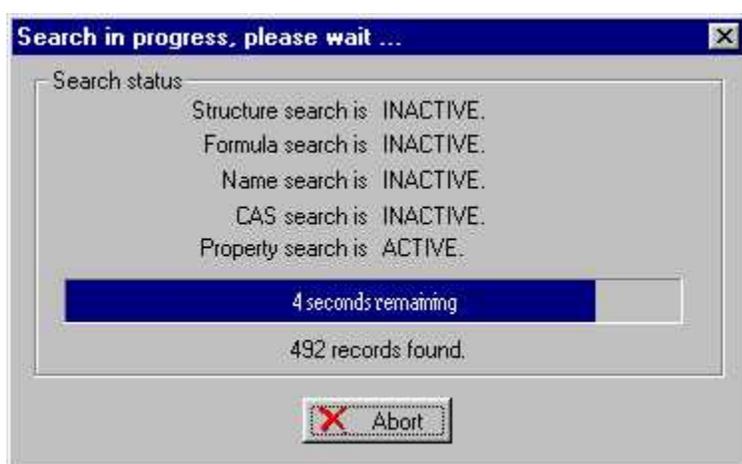


Figure 12. Search status window.

Tip: After performing a search with, for example, three simultaneous search types, if the user decides to drop one of these search types, it is best to use the “Reset” button for that field, in order to avoid searching for an empty field.

3D Viewer

In addition to the 2D Viewer of the chemical structures, automatically activated whenever there is information presented to it (for some compounds or mixtures no structure is shown), the TerraTox system has a built-in 3D Viewer. The latter can be activated at any time when there is a structure shown in the 2D viewer window by clicking on the 3D tab, shown in the enlargements in Fig. 13 (2D) and Fig. 14(3D).

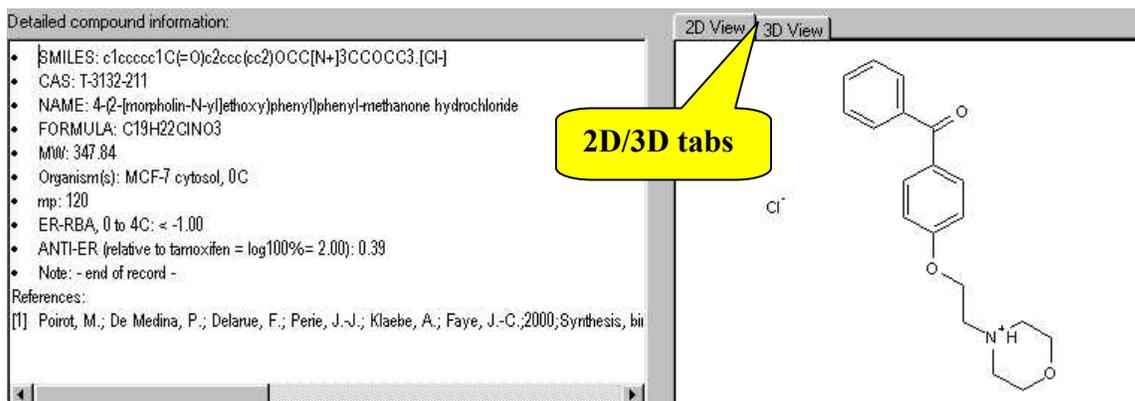


Figure 13. Detailed compound information and 2D structure.

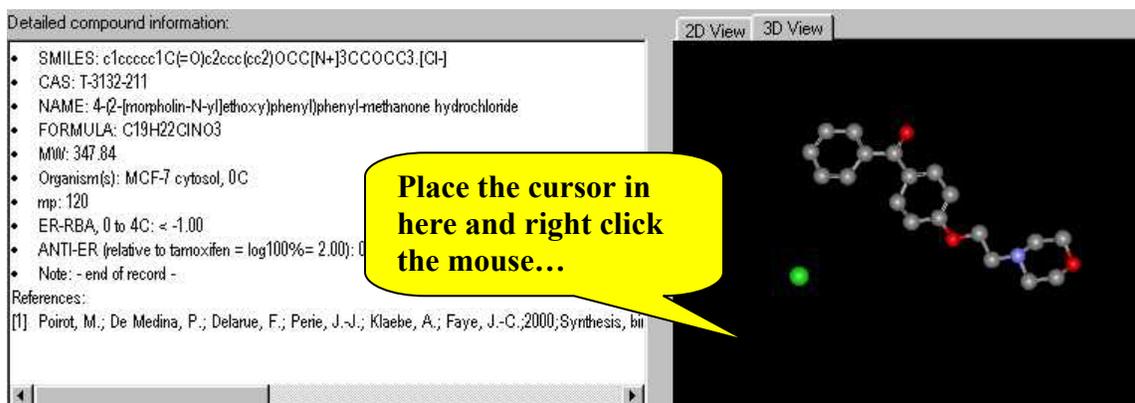


Figure 14. Detailed compound information and 3D structure (a).

The default display of the 3D display is set to “ball and stick”, but this setting can easily be changed by placing the cursor into the 3D window and using a “right click” of the mouse button. This will open a drop-down window to change the display setting, to start/stop spin of the display, etc., as shown on the same molecule in Fig. 15.

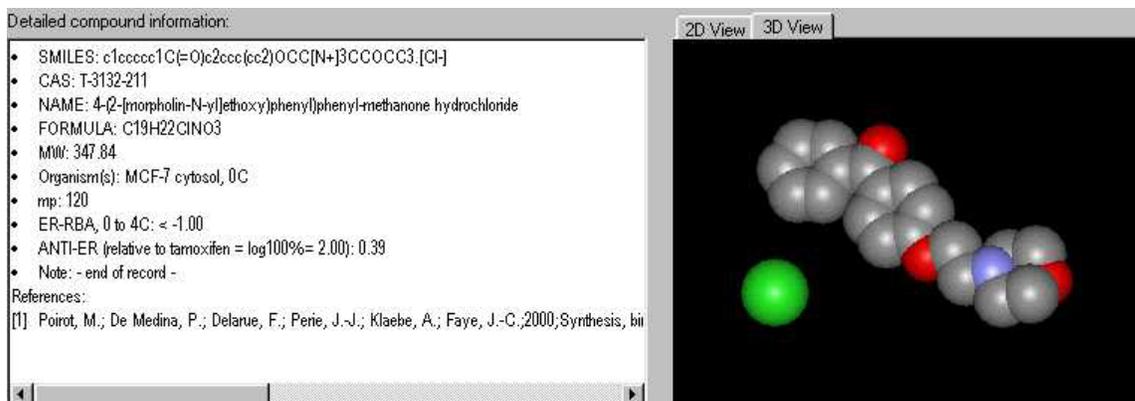


Figure 15. Detailed compound information and 3D structure (b).

In order to see a chemical structure in 3D with additional formatting, printing and file conversion capabilities, simply click on the “Details” command tab (location shown in Fig. 9). Activation of “Details” will open a new larger size window, such as shown in Fig. 16. This viewer system also has its own Help and Options system.

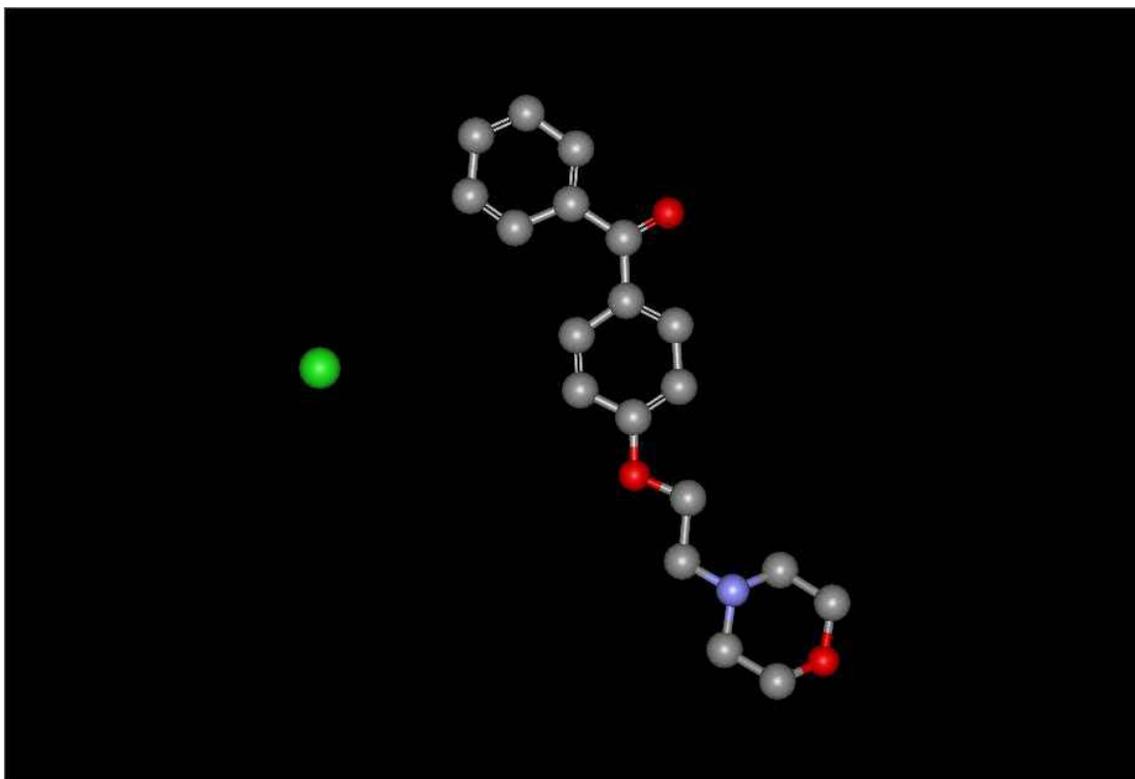


Figure 16. 3D Viewer display, accessible through the “Details” command.

Note regarding 3D structures

TerraBase Inc. cannot guarantee that 3D structures as shown in the Viewer are always displaying the correct (R or S) form of chiral (optically active) carbon atoms. While most SMILES codes in TerraTox databases have this information embedded, we have noticed that certain canonical (3D) SMILES codes are misinterpreted by the SMILES interpreter of the Viewer and get switched from one (e.g. “R”) to the other (e.g. “S”) form. For structures where the correct 3D information may be critical (such as peptide-like compounds), we recommend using a different 3D viewer, such as the ChemAxon program “MarvinView”. The latter is available for free download, after free registration, from ChemAxon, at www.chemaxon.com

In order to get the correct 3D structure picture of a canonical SMILES code provided in a TerraTox database, use the “Copy text” command and copy the entire compound information to any text editor. Then copy from there the SMILES string only, open the MarvinView program and “Edit/Paste” the SMILES string into it. In our experience, the MarvinView program has always provided the correct R/S structure information.

SMILES Notation

The Simplified Molecular Input Line Entry System (SMILES) has been developed by D. Weininger at the beginning of the 1980's. It is far superior to the previously used Wiswesser Line Notation (WLN) for coding and depicting chemical structures, by being simple, intuitive, and machine-readable. For an excellent tutorial on the SMILES notation, refer to the [Daylight Corp.](#) web site.

Recently, [Accelrys Inc.](#) introduced a variety of software modules allowing the visualization of SMILES codes as chemical structure drawings. In this process, Accelrys introduced changes to the common (Daylight Corp.) interpretation of SMILES codes by their software. As a result, lower case "c", formerly only interpreted as sp² carbon, is now interpreted as either as sp² or sp³ carbon, depending on its surrounding and connections to other atoms. The determinant here is whether or not the carbon atom is part of an aromatic ring, as defined by the Hueckel rules. This has ramifications for the correct interpretation of SMILES strings by the **TerraTox** programs, as they are built on the backbone of the Accelrys software. Therefore, all users are cautioned to ascertain that their SMILES codes follow the rules of the Accelrys software, i.e., to ascertain that only sp² carbons in ring systems which satisfy Hueckel conditions for aromaticity are given in lower case "c"; all other sp² carbons, whether in rings or not, must be entered as capital "C" together with the appropriate double bond ("=") symbols. Some examples of valid and not valid SMILES strings are listed below in Table 1.

Table 1. Valid and invalid examples of Accelrys' SMILES code

Substance	SMILES invalid	SMILES valid
cyclopentadiene ^a	<chem>c1cccC1</chem>	<chem>C1=CC=CC1</chem>
coumarin ^a	<chem>c1cc2OC(=O)ccc2cc1</chem>	<chem>c1cc2OC(=O)C=Cc2cc1</chem>

^a The SMILES strings shown as "invalid" are valid *per se*, however, the interpretation of these codes by the Accelrys system are the hydrogen-saturated compounds cyclopentane and 3,4-dihydrocoumarin, respectively.

Literature

Accelrys Inc. (2002); <http://www.accelrys.com/>.

Daylight Chemical Information Systems, Inc. (2002); SMILES Tutorial.
http://www.daylight.com/smiles/f_smiles.html.

Kaiser, K.L.E. (2003); Neural networks for effect prediction in environmental and health issues using large datasets. **QSAR Comb. Sci.**, **22**: 185-190.

Kaiser, K.L.E. (1995); Erroneous Data: Avenues for Detection and Prevention [Editorial]. **Quintessence**, **1(4)**: 13-16.

Kaiser, K.L.E. and Niculescu, S.P. (2001); On the PNN modeling of estrogen receptor binding data for carboxylic acid esters and organochlorine compounds. **Water Qual. Res. J. Canada**, **36**: 619-630 (2001); <http://www.cciw.ca/wqrjc/36-3/36-3-619.htm>.

McKinnon, M.B. and Kaiser, K.L.E. (1993); The desktop computer spreadsheet as a scientific database and powerful research tool. **Chemosphere**, **27**: 1159-1169.

Acknowledgement

TerraBase Inc. acknowledges with thanks the contributions of its contractors and associates, especially Dr. A. Krajnc and M.B. McKinnon to the development of its TerraTox products.

Security Features

As other software providers, [TerraBase Inc.](#) is interested in preventing un-authorized duplication and use of its highly sophisticated software products. Therefore, all copies of this **TerraTox** program are personalized, i.e., they contain encrypted information of the name and affiliation of the rightful user. This information is displayed on the Start-up screen and can be reviewed at any time by activating the [About](#) box, prominently displayed on the main program panel; see Figure 1. Hence, any un-authorized propagation of this software can be traced back to the original source. Anyone knowing of any such un-authorized copies is requested to contact TerraBase Inc. We offer generous rewards for information of any illegal duplication or use of this program, as described in the [About](#) box.

In order for the **TerraTox** program to function properly, the TerraTox CD has to be present in a CD-ROM drive on the computer system which is used to run the program.

Other than for archival copies, to be used solely for backup and protection against loss by the rightful user, duplication of this software is not permitted.

Legal

License Agreement

The rightful **TerraTox** user is hereby granted a non-exclusive use license, subject to the agreement as described in the text below.

TerraTox™ End User License Agreement

NOTICE TO USER: PLEASE READ THIS CONTRACT CAREFULLY. BY USING ALL OR ANY PORTION OF THE SOFTWARE YOU ACCEPT ALL THE TERMS AND CONDITIONS OF THIS AGREEMENT, INCLUDING, IN PARTICULAR THE LIMITATIONS ON: USE CONTAINED IN SECTION 2; TRANSFERABILITY IN SECTION 4; WARRANTY IN SECTION 6 AND 7; LIABILITY IN SECTION 8; AND SPECIFIC EXCEPTIONS IN SECTION 14. YOU AGREE THAT THIS AGREEMENT IS ENFORCEABLE LIKE ANY WRITTEN NEGOTIATED AGREEMENT SIGNED BY YOU. IF YOU DO NOT AGREE, DO NOT USE THIS SOFTWARE. IF YOU ACQUIRED THE SOFTWARE ON TANGIBLE MEDIA (e.g. CD) WITHOUT AN OPPORTUNITY TO REVIEW THIS LICENSE AND YOU DO NOT ACCEPT THIS AGREEMENT, YOU MAY OBTAIN A REFUND OF THE AMOUNT YOU ORIGINALLY PAID IF YOU: (A) DO NOT USE THE SOFTWARE AND (B) RETURN IT, WITH PROOF OF PAYMENT, TO THE LOCATION FROM WHICH IT WAS OBTAINED WITHIN THIRTY (30) DAYS OF THE PURCHASE DATE.

1. Definitions.

"Software" means (a) all of the contents of the files, disk(s), CD-ROM(s) or other media with which this Agreement is provided, including but not limited to (i) TerraBase Inc. or third party computer information or software; (ii) digital images, stock photographs, clip art, sounds or other artistic works ("Stock Files"); (iii) related explanatory written materials or files ("Documentation"); and (b) upgrades, modified versions, updates, additions, and copies of the Software, if any, licensed to you by TerraBase Inc. (collectively, "Updates"). "Use" or "Using" means to access, install, download, copy or otherwise benefit from using the functionality of the Software in accordance with the Documentation. "Permitted Number" means one (1) unless otherwise indicated under a valid license (e.g. volume license) granted by TerraBase Inc.. "Computer" means an electronic device that accepts information in digital or similar form and manipulates it for a specific result based on a sequence of instructions. "TerraBase" means TerraBase Inc., a Canadian corporation, 1063 King St. West, Suite 130, Hamilton, Ontario L8S 4S3, CANADA.

2. Software License.

As long as you comply with the terms of this End User License Agreement (the "Agreement"), TerraBase grants to you a non-exclusive license to Use the Software for the purposes described in the Documentation. Some third party materials included in the Software may be subject to other terms and conditions, which are typically found in a "Read Me" file located near such materials.

2.1. General Use. You may install and Use a copy of the Software solely on your compatible personal computer.

Server Use. You may not install the Software on a computer file server for the purpose of downloading, installing, or using the Software onto or with other computers.

2.3. Backup Copy. You may make one backup copy of the Software, provided your backup copy is not installed or used on any computer. You may not transfer the rights to a backup copy unless you transfer all rights in the Software as provided under Section 4.

3. Intellectual Property Rights.

The Software and any copies that you are authorized by TerraBase to make are the intellectual property of and are owned by TerraBase Incorporated and its suppliers. The structure, organization and code of the Software are the valuable trade secrets and confidential information of TerraBase Incorporated and its suppliers. The Software is protected by copyright, including without limitation by Canadian and United States Copyright Law, international treaty provisions and applicable laws in the country in which it is being

used. You may not copy the Software, except as set forth in Section 2 ("Software License"). Any copies that you are permitted to make pursuant to this Agreement must contain the same copyright and other proprietary notices that appear on or in the Software. Without exception, you agree not to modify, adapt or translate the Software. You also agree not to reverse engineer, decompile, disassemble or otherwise attempt to discover the source code of the Software. Trademarks shall be used in accordance with accepted trademark practice, including identification of trademarks owners' names. Trademarks can only be used to identify printed output produced by the Software and such use of any trademark does not give you any rights of ownership in that trademark. Except as expressly stated above, this Agreement does not grant you any intellectual property rights in the Software.

4. Transfer.

You may not rent, lease, sublicense or authorize all or any portion of the Software to be copied onto another users computer except as may be expressly permitted herein. You may, however, transfer all your rights to Use the Software to another person or legal entity provided that: (a) you also transfer each this Agreement, the Software and all other software or hardware bundled or pre-installed with the Software, including all copies, Updates and prior versions, and all copies of font software converted into other formats, to such person or entity; (b) you retain no copies, including backups and copies stored on a computer; and (c) the receiving party accepts the terms and conditions of this Agreement and any other terms and conditions upon which you legally purchased a license to the Software. Notwithstanding the foregoing, you may not transfer education, pre-release, or not for resale copies of the Software.

5. Updates.

If the Software is an Update to a previous version of the Software, you must possess a valid license to such previous version in order to Use the Update. You may continue to Use the previous version of the Software on your computer after you receive the Update to assist you in the transition to the Update, provided that: the Update and the previous version are installed on the same computer; the previous version or copies thereof are not transferred to another party or computer unless all copies of the Update are also transferred to such party or computer; and you acknowledge that any obligation TerraBase may have to support the previous version of the Software may be ended upon availability of the Update.

6. LIMITED WARRANTY.

Except as may be otherwise provided in Section 14, TerraBase warrants to the person or entity that first purchases a license for the Software for use pursuant to the terms of this license, that the Software will perform substantially in accordance with the Documentation for the ninety (90) day period following receipt of the Software when used on the recommended hardware configuration. Non-substantial variations of performance from the Documentation does not establish a warranty right. THIS LIMITED WARRANTY DOES NOT APPLY TO UPDATES, FONT SOFTWARE CONVERTED INTO OTHER FORMATS, PRE-RELEASE (BETA), TRYOUT, PRODUCT SAMPLER, OR NOT FOR RESALE (NFR) COPIES OF SOFTWARE (See Section 14). To make a warranty claim, you must return the Software to the location where you obtained it along with proof of purchase within such ninety (90) day period. If the Software does not perform substantially in accordance with the Documentation, the entire liability of TerraBase and your exclusive remedy shall be limited to either, at TerraBase's option, the replacement of the Software or the refund of the license fee you paid for the Software. THE LIMITED WARRANTY SET FORTH IN THIS SECTION GIVES YOU SPECIFIC LEGAL RIGHTS. YOU MAY HAVE ADDITIONAL RIGHTS WHICH VARY FROM JURISDICTION TO JURISDICTION. For further warranty information, please see the jurisdiction specific information at the end of this Agreement, if any, or contact TerraBase.

7. DISCLAIMER.

THE FOREGOING LIMITED WARRANTY STATES THE SOLE AND EXCLUSIVE REMEDIES FOR TERRABASE'S OR ITS SUPPLIER'S BREACH OF WARRANTY. TERRABASE AND ITS SUPPLIERS DO NOT AND CANNOT WARRANT THE PERFORMANCE OR RESULTS YOU MAY OBTAIN BY USING THE SOFTWARE. EXCEPT FOR THE FOREGOING LIMITED WARRANTY, AND FOR ANY WARRANTY, CONDITION, REPRESENTATION OR TERM TO THE EXTENT TO WHICH THE SAME CANNOT OR MAY NOT BE EXCLUDED OR LIMITED BY LAW APPLICABLE TO YOU IN YOUR JURISDICTION, TERRABASE AND ITS SUPPLIERS MAKE NO WARRANTIES, CONDITIONS, REPRESENTATIONS OR TERMS, EXPRESS OR IMPLIED, WHETHER BY STATUTE, COMMON LAW, CUSTOM, USAGE OR OTHERWISE AS TO ANY OTHER MATTERS, INCLUDING BUT NOT LIMITED TO NON-INFRINGEMENT OF THIRD PARTY RIGHTS, INTEGRATION, SATISFACTORY QUALITY OR FITNESS FOR ANY PARTICULAR PURPOSE. The provisions of this section 7 shall survive the termination of this Agreement, howsoever caused, but this shall not imply or create

any continued right to Use the Software after termination of this Agreement.

8. LIMITATION OF LIABILITY.

IN NO EVENT WILL TERRABASE OR ITS SUPPLIERS BE LIABLE TO YOU FOR ANY DAMAGES, CLAIMS OR COSTS WHATSOEVER OR ANY CONSEQUENTIAL, INDIRECT, INCIDENTAL DAMAGES, OR ANY LOST PROFITS OR LOST SAVINGS, EVEN IF AN TERRABASE REPRESENTATIVE HAS BEEN ADVISED OF THE POSSIBILITY OF SUCH LOSS, DAMAGES, CLAIMS OR COSTS OR FOR ANY CLAIM BY ANY THIRD PARTY. THE FOREGOING LIMITATIONS AND EXCLUSIONS APPLY TO THE EXTENT PERMITTED BY APPLICABLE LAW IN YOUR JURISDICTION. TERRABASE'S AGGREGATE LIABILITY AND THAT OF ITS SUPPLIERS UNDER OR IN CONNECTION WITH THIS AGREEMENT SHALL BE LIMITED TO THE AMOUNT PAID FOR THE SOFTWARE, IF ANY. Nothing contained in this Agreement limits TerraBase's liability to you in the event of death or personal injury resulting from TerraBase's negligence or for the tort of deceit (fraud). TerraBase is acting on behalf of its suppliers for the purpose of disclaiming, excluding and/or limiting obligations, warranties and liability as provided in this Agreement, but in no other respects and for no other purpose. For further information, please see the jurisdiction specific information at the end of this Agreement, if any, or contact TerraBase.

9. Export Rules. You agree that the Software will not be shipped, transferred or exported into any country or used in any manner prohibited by the any law governing such activities either in Canada or the United States, such as the United States Export Administration Act or any other export laws, restrictions or regulations (collectively the "Export Laws"). In addition, if the Software is identified as export controlled items under the Export Laws, you represent and warrant that you are not a citizen, or otherwise located within, an embargoed nation (including without limitation Iran, Iraq, Syria, Sudan, Libya, Cuba, North Korea, and Serbia) and that you are not otherwise prohibited under the Export Laws from receiving the Software. All rights to Use the Software are granted on condition that such rights are forfeited if you fail to comply with the terms of this Agreement.

10. Governing Law.

This Agreement will be governed by and construed in accordance with the substantive laws in force: (a) the Province of Ontario, if the license to the Software is purchased when you are in Canada, the United States, Canada, or Mexico; or (b) in Japan, if a license to the Software is purchased when you are in Japan, China, Korea, R.O.C, or other Southeast Asian country where all official languages are written in either an ideographic script (e.g., hanzi, kanji, or hanja), and/or other script based upon or similar in structure to an ideographic script, such as hangul or kana; or (c) the Netherlands, if a license to the Software is purchased when you are in any other jurisdiction not described above. The respective courts of Ontario when Canadian law applies, Tokyo District Court in Japan, when Japanese law applies, and the courts of Amsterdam, the Netherlands, when the law of the Netherlands applies, shall each have non-exclusive jurisdiction over all disputes relating to this Agreement. This Agreement will not be governed by the conflict of law rules of any jurisdiction or the United Nations Convention on Contracts for the International Sale of Goods, the application of which is expressly excluded.

11. General Provisions.

If any part of this Agreement is found void and unenforceable, it will not affect the validity of the balance of the Agreement, which shall remain valid and enforceable according to its terms. This Agreement shall not prejudice the statutory rights of any party dealing as a consumer. This Agreement may only be modified by a writing signed by an authorized officer of TerraBase. Updates may be licensed to you by TerraBase with additional or different terms. This is the entire agreement between TerraBase and you relating to the Software and it supersedes any prior representations, discussions, undertakings, communications or advertising relating to the Software.

12. Notice to U.S. Government End Users.

The Software and Documentation are "Commercial Items," as that term is defined at 48 C.F.R. §2.101, consisting of "Commercial Computer Software" and "Commercial Computer Software Documentation," as such terms are used in 48 C.F.R. §12.212 or 48 C.F.R. §227.7202, as applicable. Consistent with 48 C.F.R. §12.212 or 48 C.F.R. §§227.7202-1 through 227.7202-4, as applicable, the Commercial Computer Software and Commercial Computer Software Documentation are being licensed to U.S. Government end users (a) only as Commercial Items and (b) with only those rights as are granted to all other end users pursuant to the terms and conditions herein. Unpublished-rights reserved under the copyright laws of the United States by TerraBase Incorporated, 1063 King St. West, Suite 130, Hamilton, Ontario L8S 4S3, CANADA.

13. Compliance with Licenses.

If you are a business or organisation, you agree that upon request from TerraBase or TerraBase's authorised representative, you will within thirty (30) days fully document and certify that use of any and all TerraBase Software at the time of the request is in conformity with your valid licenses from TerraBase.

14. SPECIFIC EXCEPTIONS.

14.1 Limited Warranty for Users Located in Germany or Austria. If you purchased a license to the software in Germany or Austria then Section 6 does not apply, instead, TerraBase warrants to the person or entity that first purchases a license for the Software, that the Software will perform substantially in accordance with the Documentation for a period of six (6) months following receipt of the Software when used on the recommended hardware configuration. Non-substantial variations of performance from the Documentation does not establish a warranty right. THIS LIMITED WARRANTY DOES NOT APPLY TO UPDATES, FONT SOFTWARE CONVERTED INTO OTHER FORMATS, PRE-RELEASE, TRYOUT, PRODUCT SAMPLER, NOT FOR RESALE (NFR) COPIES OF SOFTWARE, OR TO SOFTWARE THAT HAS BEEN ALTERED BY YOU, TO THE EXTENT SUCH ALTERATIONS CAUSED A DEFECT. To make a warranty claim, you must return the Software, at our expense, to the location where you obtained it along with proof of purchase within such six (6) month period. If the Software does not perform substantially in accordance with the Documentation, the entire liability of TerraBase and your exclusive remedy shall be limited to either, at TerraBase's option, the replacement of the Software, the reduction of the license fee, or a refund of the license fee you paid for the Software. THE LIMITED WARRANTY SET FORTH IN THIS SECTION GIVES YOU SPECIFIC LEGAL RIGHTS. For further warranty information, please contact TerraBase.

14.2 Limitation of Liability for Users Located in Germany and Austria. If you purchased a license to the software in Germany or Austria then Section 8 does not apply, instead, TerraBase may be liable without limitation for damages you have incurred under or in connection with this Agreement only if the damage has been caused by the willful or grossly negligent act of TerraBase or its agents. TerraBase is liable only to the extent of the typically foreseeable damage for such damages which have been caused by any other negligent breach of a substantial contractual duty by TerraBase or its agents. These aforementioned limitations apply irrespective of their legal basis, in particular with regard to any pre-contractual or auxiliary contractual claims. The limitations shall not apply, however, to any mandatory liability under the applicable German or Austrian Product Liability Act, nor to any damage which is caused due to the breach of an express warranty to the extent that such express warranty was intended to protect the user against the specific damage incurred. The obligations under the second sentence shall not apply if any damage is caused by your having altered the Software, or if the respective data carriers (media) have been damaged by accident, misuse or inappropriate use, or if the damage concerned has been caused by the use of the Software in connection with other software for which the Software was not designated to be used according to the Documentation.

14.3 Pre-release Product Additional Terms. If the product you have received with this license is pre-commercial release or beta Software ("Pre-release Software"), then the following Section applies. To the extent that any provision in this Section is in conflict with any other term or condition in this Agreement, this Section shall supercede such other term(s) and condition(s) with respect to the Pre-release Software, but only to the extent necessary to resolve the conflict. You acknowledge that the Software is a pre-release version, does not represent final product from TerraBase, and may contain bugs, errors and other problems that could cause system or other failures and data loss. Consequently, the Pre-release Software is provided to you "AS-IS", and TerraBase disclaims any warranty or liability obligations to you of any kind. WHERE LEGALLY LIABILITY CANNOT BE EXCLUDED FOR PRE-RELEASE SOFTWARE, BUT IT MAY BE LIMITED, TERRABASE'S LIABILITY AND THAT OF ITS SUPPLIERS SHALL BE LIMITED TO THE SUM OF FIFTY DOLLARS (U.S. \$50) IN TOTAL. You acknowledge that TerraBase has not promised or guaranteed to you that Pre-release Software will be announced or made available to anyone in the future, that TerraBase has no express or implied obligation to you to announce or introduce the Pre-release Software and that TerraBase may not introduce a product similar to or compatible with the Pre-release Software. Accordingly, you acknowledge that any research or development that you perform regarding the Pre-release Software or any product associated with the Pre-release Software is done entirely at your own risk. During the term of this Agreement, if requested by TerraBase, you will provide feedback to TerraBase regarding testing and use of the Pre-release Software, including error or bug reports. If you have been provided the Pre-release Software pursuant to a separate written agreement, such as the TerraBase Incorporated Serial Agreement for Unreleased Products, your use of the Software is also governed by such agreement. You agree that you may not and certify that you will not sublicense, lease, loan, rent, or transfer

the Pre-release Software. Upon receipt of a later unreleased version of the Pre-release Software or release by TerraBase of a publicly released commercial version of the Software, whether as a stand-alone product or as part of a larger product, you agree to return or destroy all earlier Pre-release Software received from TerraBase and to abide by the terms of the End User License Agreement for any such later versions of the Pre-release Software. Notwithstanding anything in this Section to the contrary, if you are located outside Canada or the United States of America, you agree that you will return or destroy all unreleased versions of the Pre-release Software within thirty (30) days of the completion of your testing of the Software when such date is earlier than the date for TerraBase's first commercial shipment of the publicly released (commercial) Software.

14.4 Tryout, Product Sampler, NFR, Additional Terms. If the product you have received with this license is a tryout, product sampler, or NFR copy of the Software ("Tryout Software"), then the following Section applies until such time that you purchase a license to the full retail version of such product. To the extent that any provision in this Section is in conflict with any other term or condition in this Agreement, this Section shall supercede such other term(s) and condition(s) with respect to the Tryout Software, but only to the extent necessary to resolve the conflict. YOU ACKNOWLEDGE THAT THE TRYOUT SOFTWARE CONTAINS LIMITED FUNCTIONALITY AND/OR FUNCTIONS FOR A LIMITED PERIOD OF TIME. TERRABASE IS LICENSING THE SOFTWARE ON AN "AS IS" BASIS, SOLELY AS A DEMONSTRATION MODEL. If the Tryout Software is a timeout version, then the program will terminate operations after a designated period of time (e.g. 15. 30. or 45 days) following installation (the "Time Out Date"), which is specified in the Software. Upon such Time Out Date, the license hereunder shall be terminated, unless extended by TerraBase upon your purchase of a full retail license from TerraBase. You acknowledge that such Tryout Software shall cease operation upon the Time Out Date and accordingly, access to any files or output created with such Tryout Software or any product associated with the Tryout Software is done entirely at your own risk. TERRABASE DISCLAIMS ANY WARRANTY OR LIABILITY OBLIGATIONS TO YOU OF ANY KIND, INCLUDING, WHERE LEGALLY LIABILITY CANNOT BE EXCLUDED FOR PRE-RELEASE SOFTWARE, BUT IT MAY BE LIMITED, TERRABASE'S LIABILITY AND THAT OF ITS SUPPLIERS SHALL BE LIMITED TO THE SUM OF FIFTY DOLLARS (U.S. \$50) IN TOTAL.

15. This concludes the License Agreement for the TerraTox software. If you have any questions regarding this Agreement or if you wish to request any information from TerraBase please use the address and contact information included with this product to contact TerraBase.

Gen_WWCombined_USEnglish_8.7.00_11:14

Trademarks and Copyrights

Windows 95, Windows 98, Windows NT, Windows 2000, Windows ME, and Windows XP are trademarks of Microsoft Corporation, Redmond, Washington, USA. Other copyrights and trademarks are those of their respective owners.

Technical Requirements

Operating system: PC with Windows 98, NT, 2000, ME, or XP operating system.

Central processor unit (CPU): No specific requirement, duration of searches will vary with hard disk and CPU speed; 2.0 GHz or higher CPU recommended.

Mouse or other pointing device: required.

Screen setting: Variable, 800 x 640, or higher recommended.

CD-ROM drive: required.

Other: Presence of the TerraTox CD in the CD-ROM drive is required for program execution.

Installation Instructions

The **TerraTox** software is a fully functional, stand-alone system, easy to install or uninstall. It consists of four installation parts; we recommend installation in the order given below. Before proceeding with the installation, please print the **Readme.txt** file in the root directory of the TerraTox CD for important installation information and carefully follow the recommendations given therein.

Part 1. Adobe software

To install the Adobe Reader program (vs. 5.05), which is required to read the TerraTox Manual (accessible from the “F1” key, or from the “TerraTox Help” menu), use the Windows – Control – Install/Remove Software command to run the “ar505enu.exe” in the Adobe folder and follow the instructions.

Part 2. Accelrys software

To install/un-install the Accelrys supporting software, necessary for the proper functioning of the **TerraTox** program, use the Windows – Control – Install/Remove Software command to run each of the “exe” files in the Accelrys folder. See the **Readme.txt** file for detailed installation instructions.

Part 3. Viewer software

To install/un-install Viewer supporting software, necessary for the proper functioning of the **TerraTox** program, use the Windows – Control – Install/Remove Software command to run each of the “exe” files in the Viewer folder. See the **Readme.txt** file for detailed installation instructions.

Part 4. TerraTox software

To install/un-install the **TerraTox** software, follow the instructions in the **Readme.txt** file.

Customer Support

[TerraBase Inc.](#) is committed to effective customer support. With the rapid change in PC technology, operating systems and other software and hardware changes, the occasional hiccup is bound to happen. We will try our best to help customers with problems related to our products, in most cases free of charge. Contact our help department with any question and concern about our products, either by EMAIL, FAX, or MAIL.

TerraBase Inc.
1063 King St. West, Suite 130
Hamilton, ON, L8S 4S3, Canada
Fax: 905-527-0263
Internet: <http://www.terrabase.ca>