TerraTox™ Databases
User Manual, vs. 3.5

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 ~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™ - Aqua
TerraTox™ - Antimalarials
TerraTox™ - COX (Cyclooxygenase inhibitors)
TerraTox™ - Critical Data
TerraTox™ - Drugs
TerraTox™ - Dyes
TerraTox™ - Explorer
TerraTox™ - Fragrances
TerraTox™ - HBEE
TerraTox™ - HIV-1
TerraTox™ - Ionic Liquids
TerraTox™ - Natural Products
TerraTox™ - Pesticides
TerraTox™ - Skin
TerraTox™ - Steroids-RBA
TerraTox™ - Surfactants & Chelators
TerraTox™ - *Tetrahymena*
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.

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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 and biology.

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.

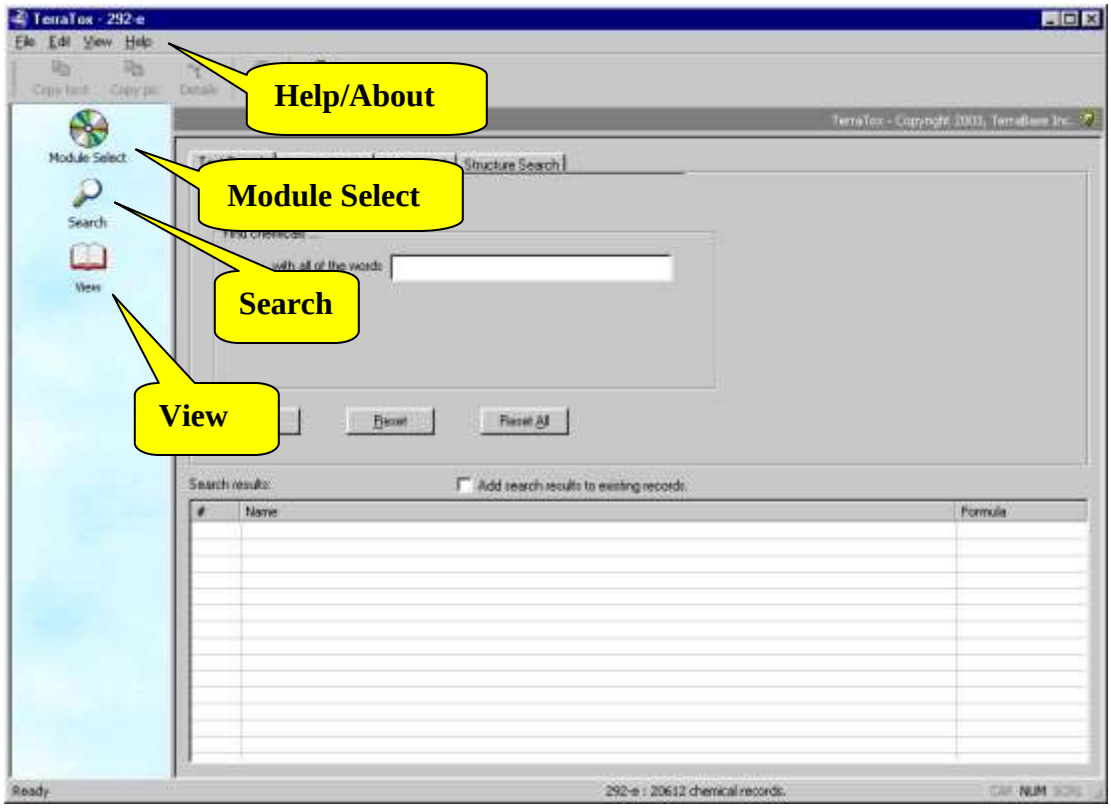

Figure 1. TerraTox opening window.

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.

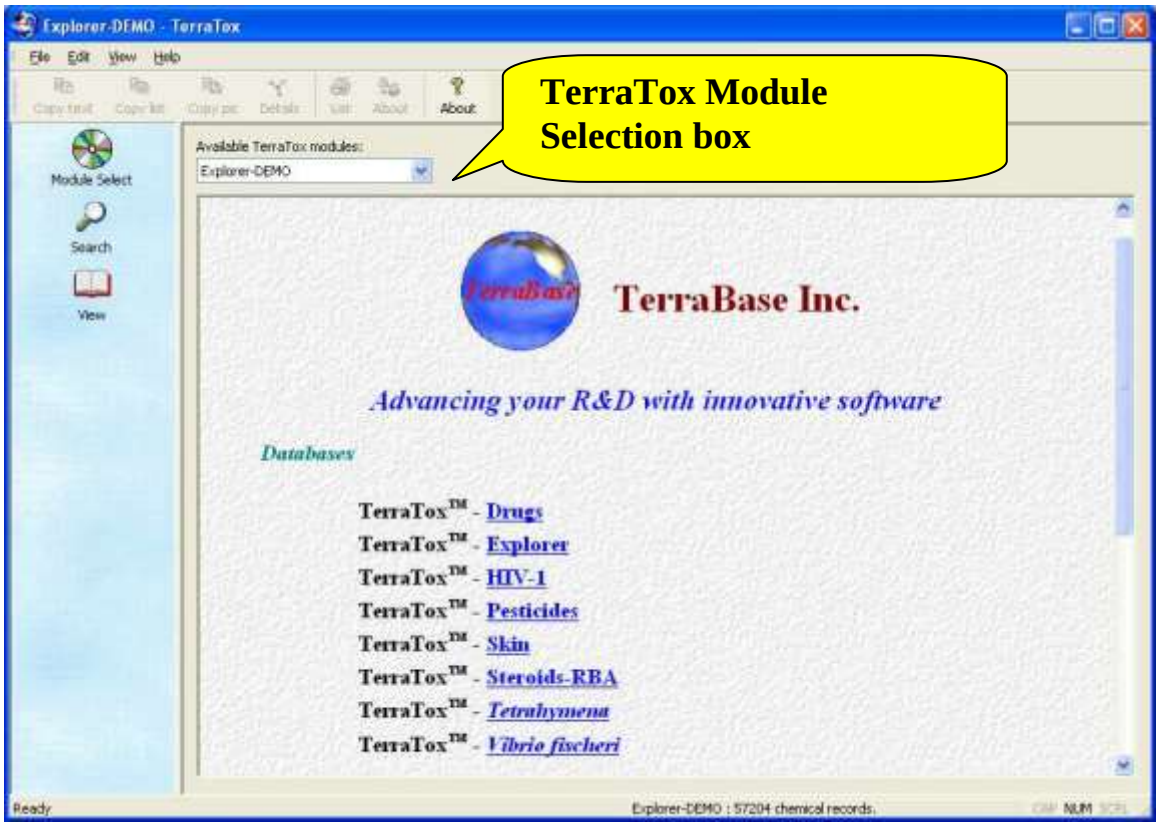

Figure 2. Module Selection box.

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 five search capabilities of TerraTox databases.

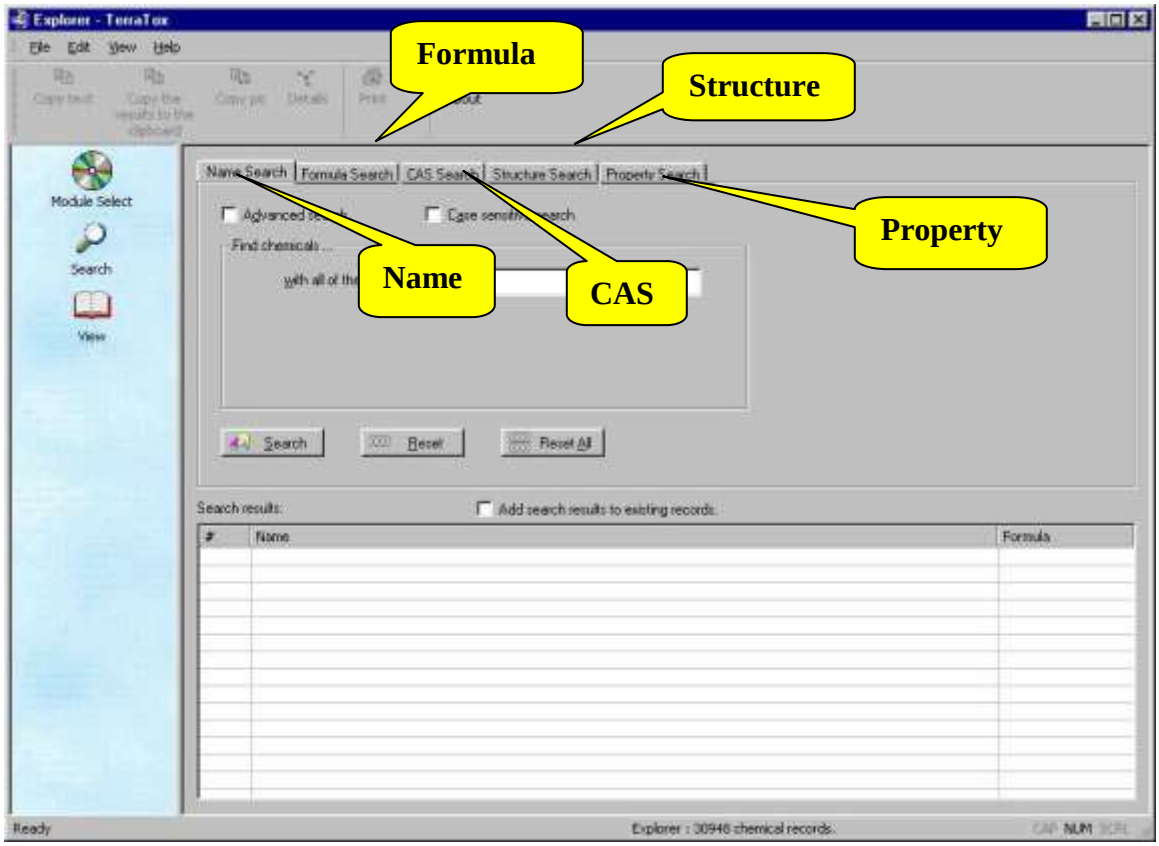

Figure 3. Search window overview.

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.

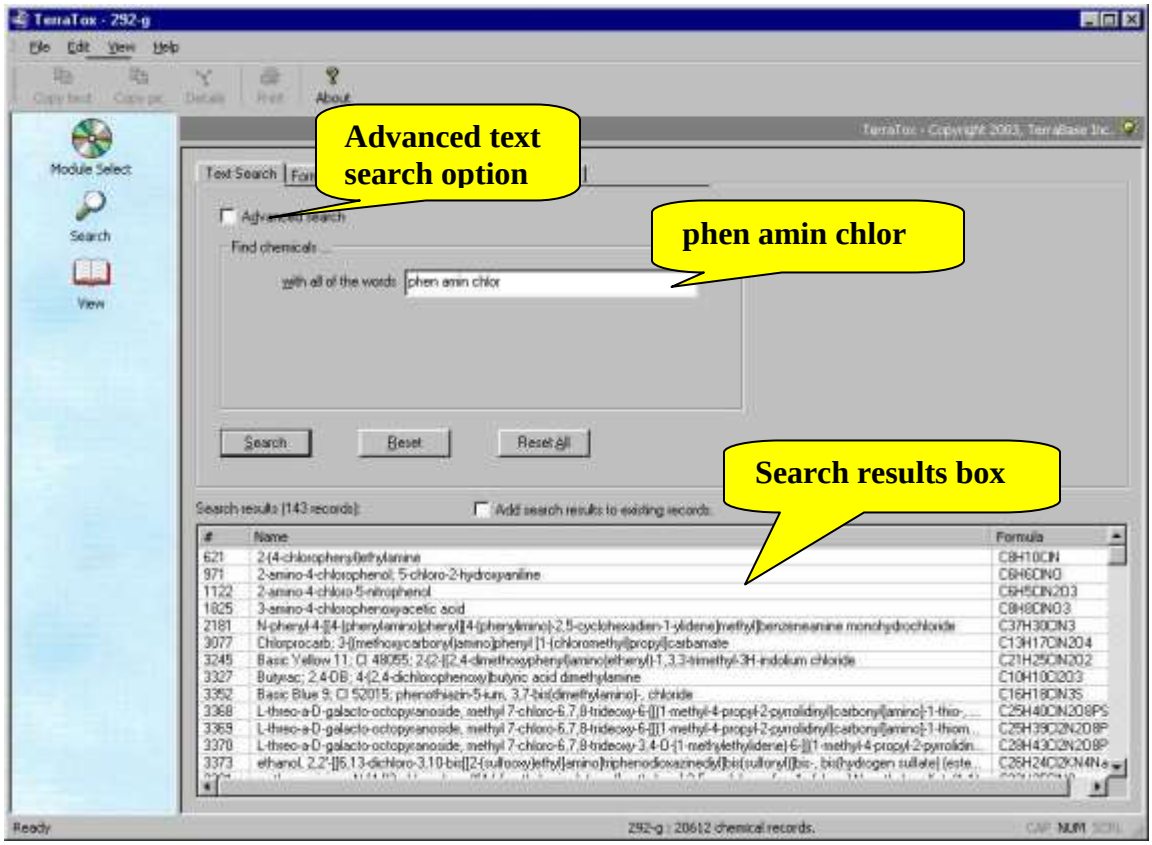

Figure 4. Standard Name search.

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.

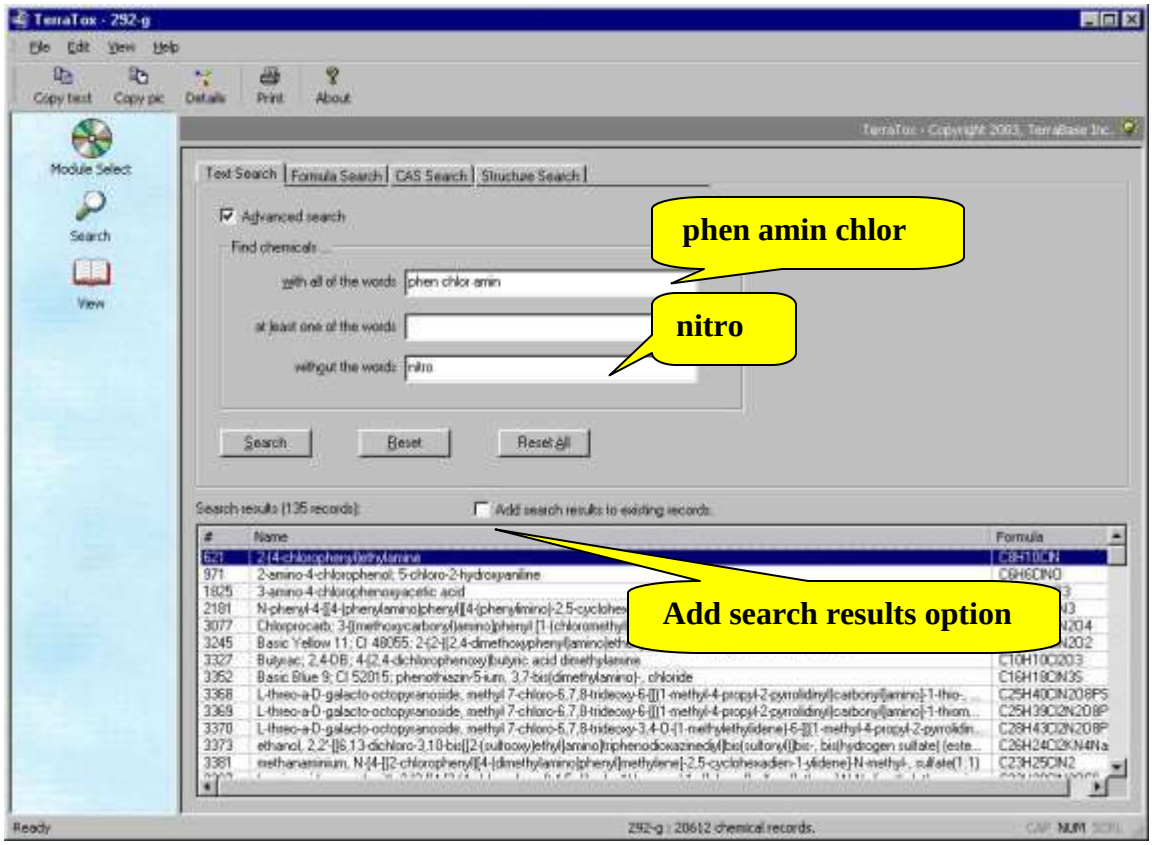

Figure 5. Advanced Name search.

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".

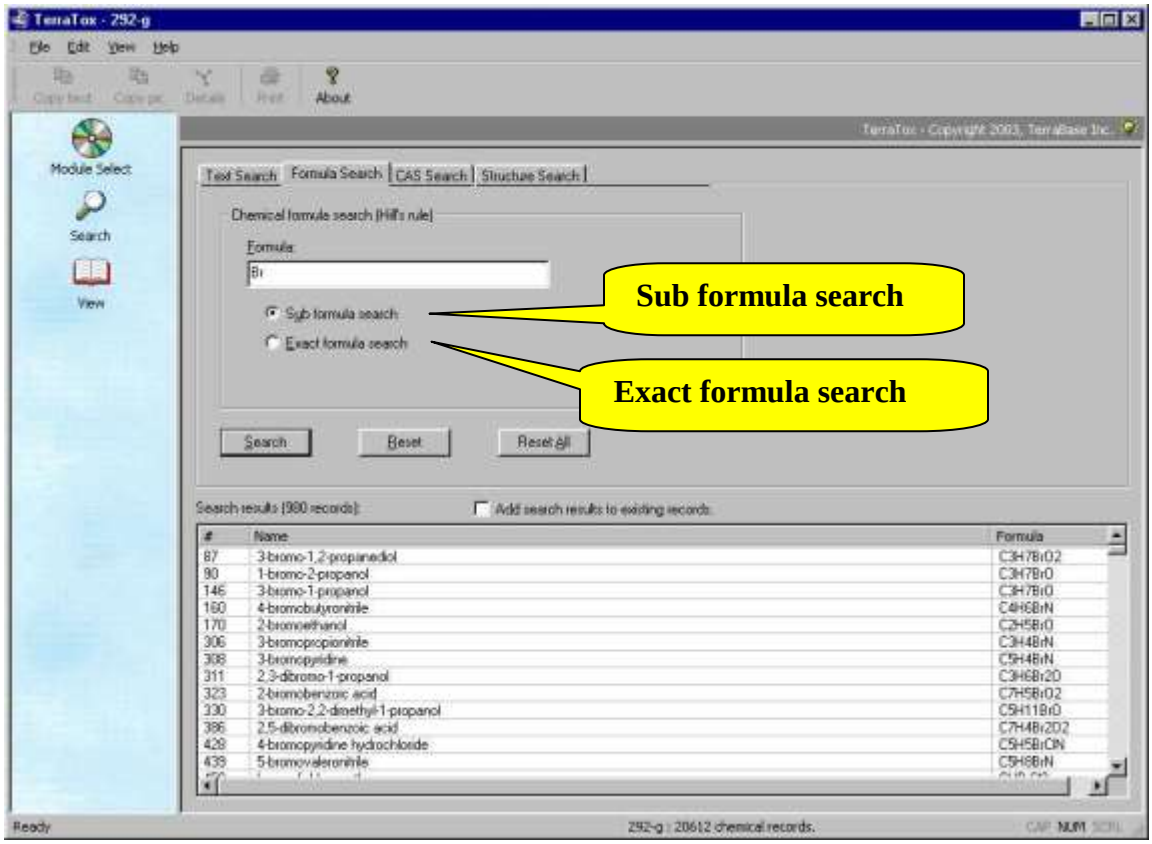

Figure 6. Formula Search window.

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.

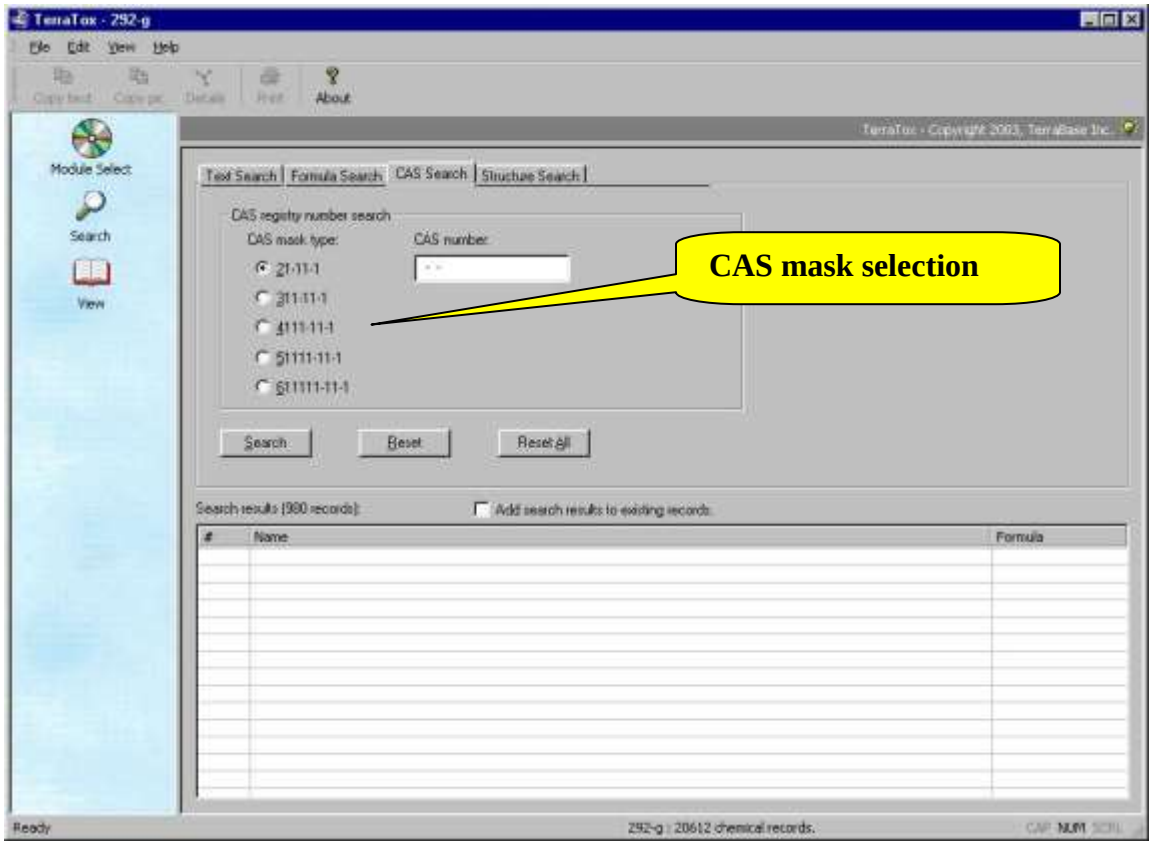

Figure 7. CAS Search window.

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.

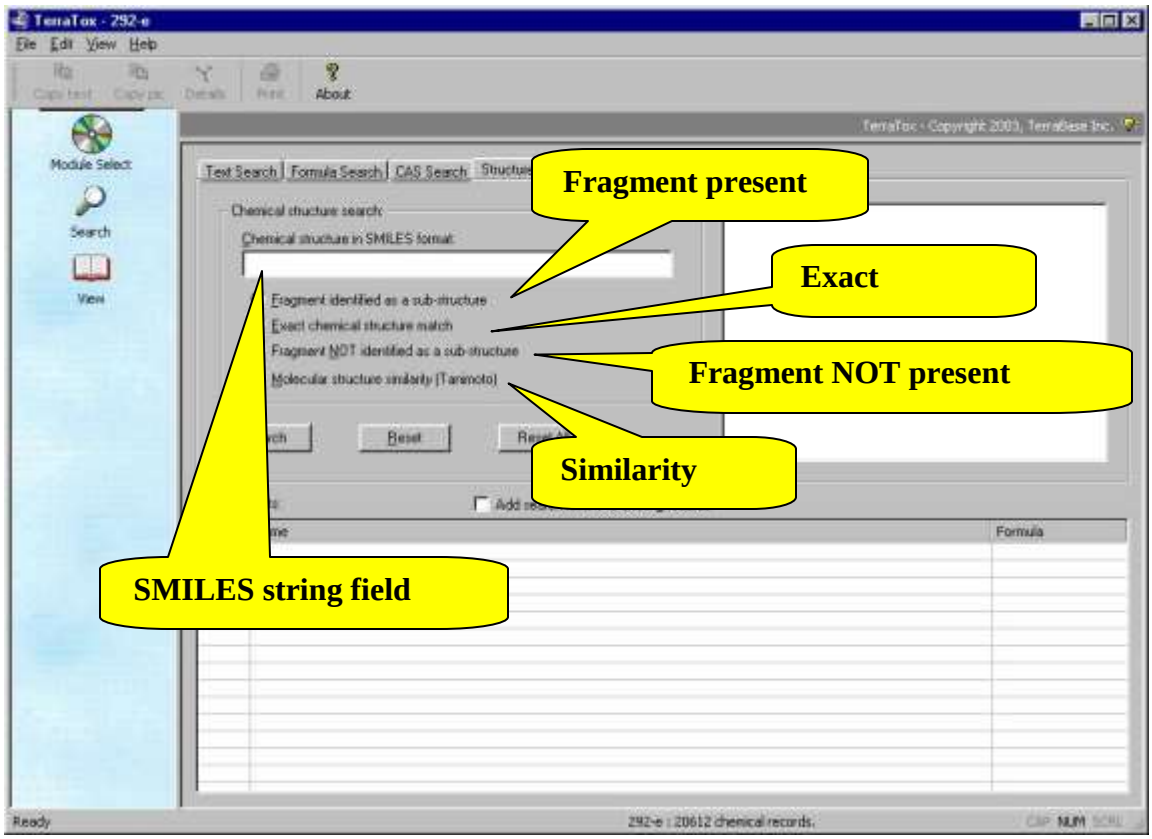

Figure 8. Chemical structure search window.

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.

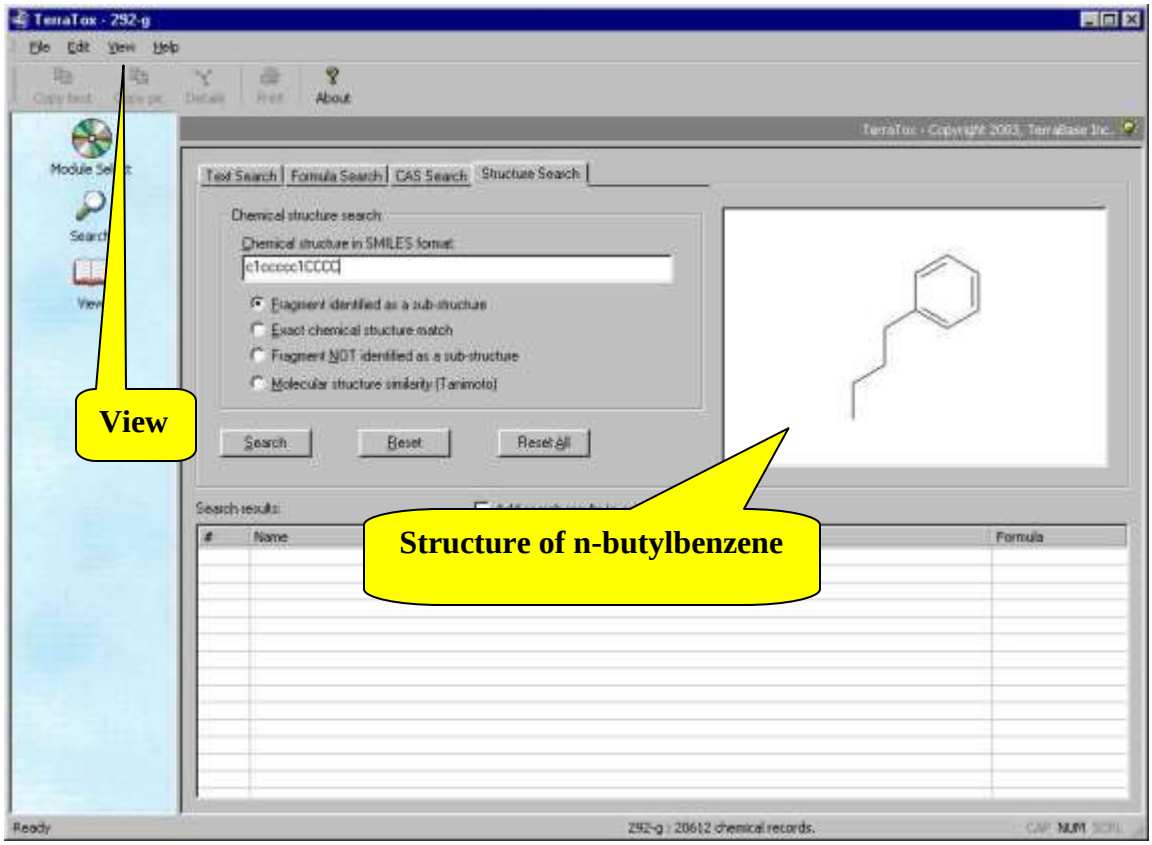

Figure 9. Chemical structure search window with SMILES string.

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 ("<=").

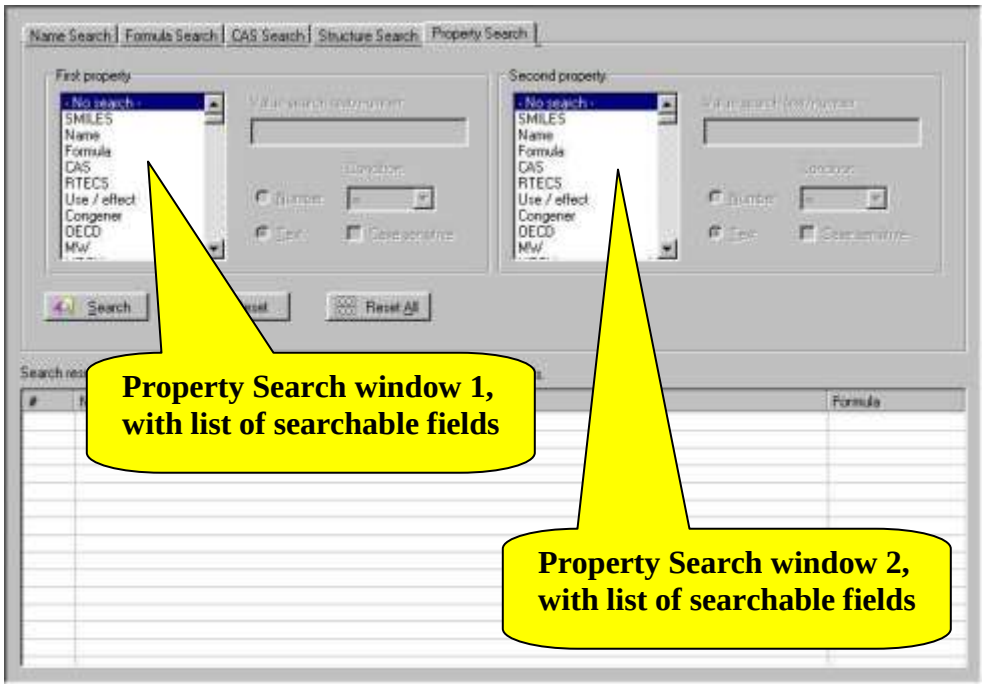

Figure 10. Property search window.

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.

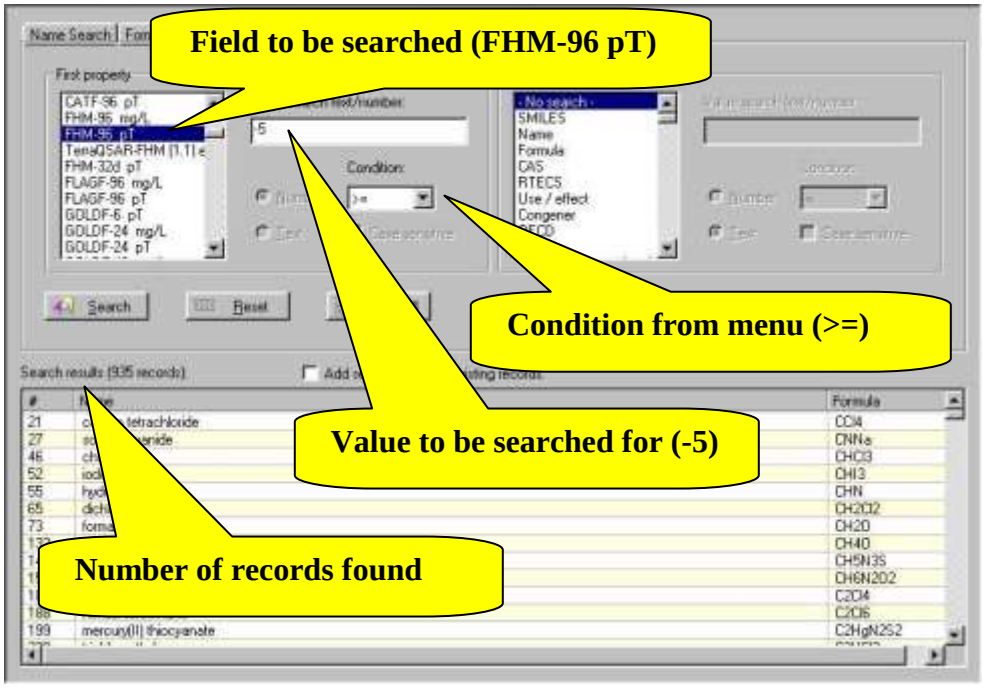

Figure 11. Property search result.

Property searches can be done on any field but the references. For a current list of covered properties and effects, please consult the file "**TerraTox-Parameters.htm**" available in the root directory of the CD.

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).

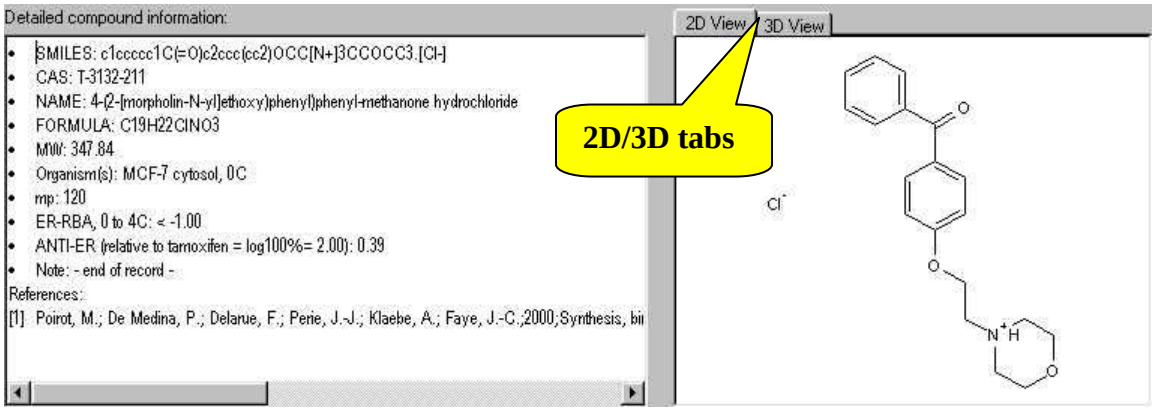

Figure 13. Detailed compound information and 2D structure.

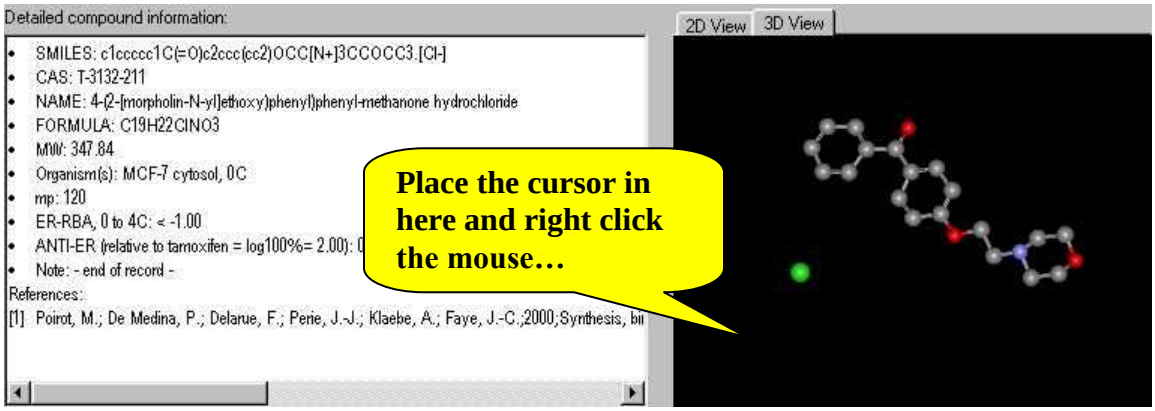

Figure 14. Detailed compound information and 3D structure (a).

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.

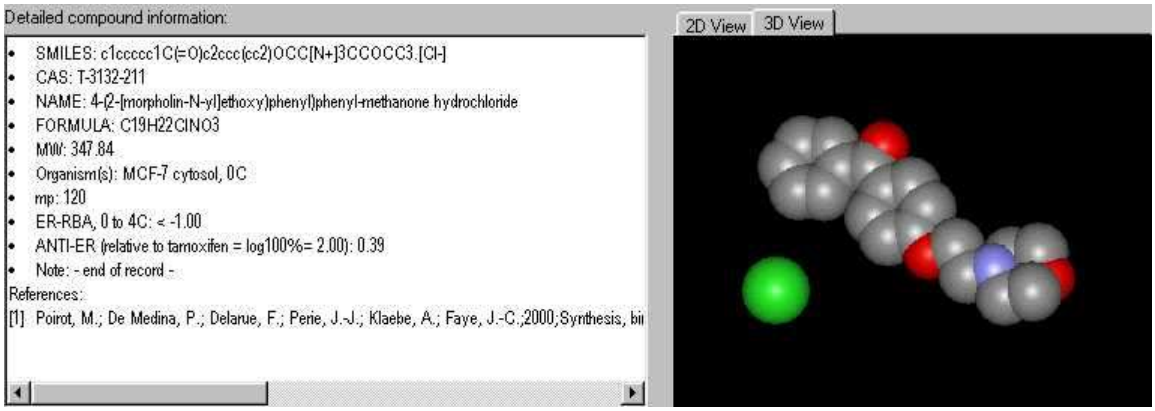

Figure 15. Detailed compound information and 3D structure (b).

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.

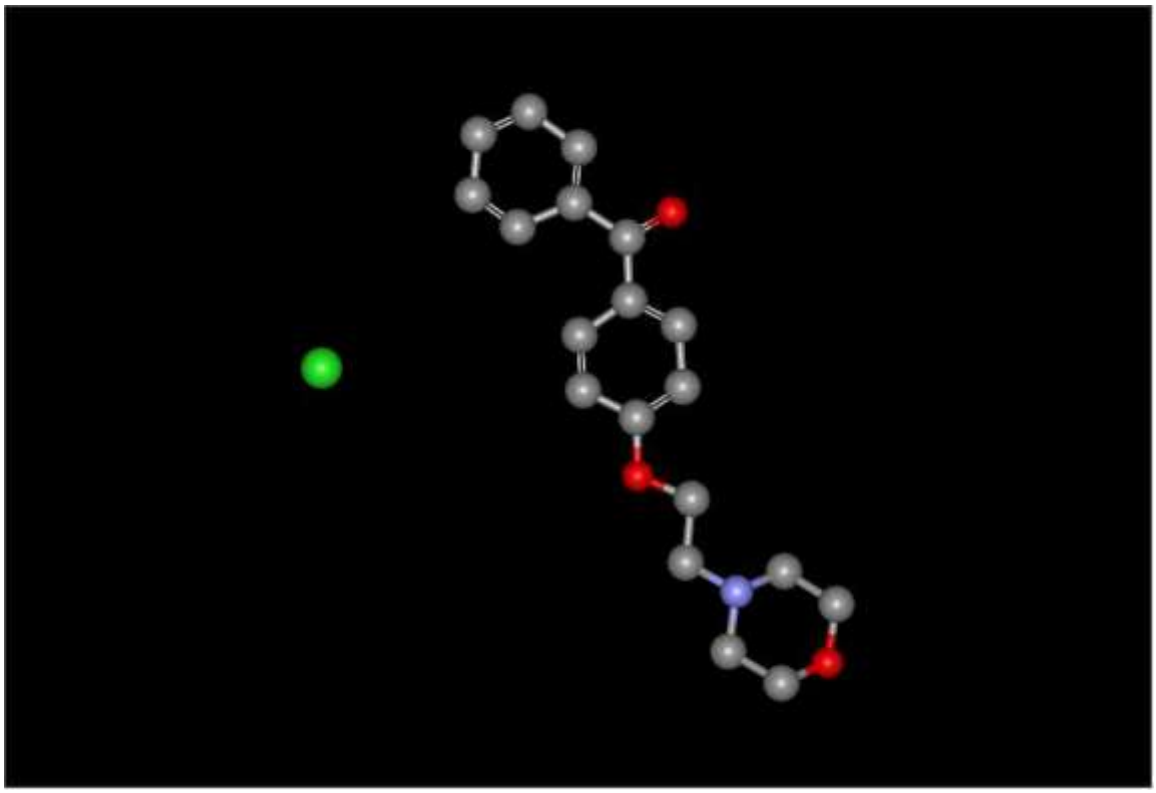

Figure 16. 3D Viewer display, accessible through the "Details" command.

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 sp^2 carbon, is now interpreted as either as sp^2 or sp^3 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 sp^2 carbons in ring systems which satisfy Hueckel conditions for aromaticity are given in lower case "c"; all other sp^2 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]	c1cccC1	C1=CC=CC1
coumarin [a]	c1cc2OC(=O)ccc2cc1	c1cc2OC(=O)C=Cc2cc1

[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

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As other software providers, TerraBase Inc. is interested is 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.

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Technical Requirements

Operating system: PC with Windows 98, NT, 2000, ME, or XP (SP2), Vista, XP, 7, and 10 operating systems, including 64-bit systems.
Central processor unit (CPU): No specific requirement, duration of searches will vary with hard disk and CPU speed; 4.0 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. Acrobat software

To install the Acrobat Reader program (vs. 7.0), 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 "AdbeRdr70_enu_full.exe" in the Acrobat 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, follow the instructions in the README file.

Part 3. Viewer software

Follow the instructions in the README file.

Part 4. TerraTox software

To install the **TerraTox** software, double click on the "TerraTox-Setup.exe" file in the root directory, using the communicated password.

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