VERSION 0.8.4

USER GUIDE

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1. Introduction

ToxEraser Solvents is a software designed with the aim to identify risky solvents and suggest safer alternatives as remedy. The first component of the tool is represented by an archive consisting of relevant lists and databases, which are described in detail in the Appendix I of this user guide. They are all drafted by panel of experts working on chemical risk assessment, from industry, academia and regulatory agencies. By assuming the selected lists as a source of independent information, the systematic evaluation of what resulted from their assessment was meant to offer a comprehensive classification of solvents, at least in comparison with the classification endorsed by each single list. The procedure applied to develop the final safety classes is described in the Appendix II of this user guide. Moreover, a read-across analysis enforces the substitution process, making the substitution possible even when the ingredient is not included in the archive. Finally, a series of structural alerts have been implemented in order to detect possible evidence of toxicity for different toxicological endpoints. The structural alerts implemented within the tools are: Benigni-Bossa ruleset for carcinogenicity and mutagenicity (from Toxtree), Endocrine disruptors alerts developed by IRFMN considering EU and WHO lists and aquatic toxicity alerts developed by IRFMN.
ToxEraser Solvents works with a single ingredient, entered by the end user in the Graphical User Interface (GUI).
ToxEraser Solvents is a Java standalone application. It has been designed with flexible capabilities for future extension in mind (possibility to add new lists of ingredients or set new functionalities).

2. Installing and starting ToxEraser Solvents

ToxEraser Solvents is a JAVA application that works on every operating system (Windows/Linux/Mac) supporting Java. Before proceeding, please check what version of Java is installed in your OS and if the JAVA_PATH environment variable is correctly set (for further details, please refer to Oracle documentation https://docs.oracle.com/cd/E19182-01/821-0917/inst_jdk_javahome_t/index.html).

ToxEraser Solvents works with Java 8 or OpenJDK Java 11+: depending on what version is installed or set in your operative system please follow the instructions below:

WINDOWS:

- **JAVA 8:** Download and unpack the zipped file. To start the application, move to the application folder and run the file *starter.bat*
- **OPEN JDK JAVA 11 or greater**: Download and unpack the zipped file. To start the application, you can just run the file *ToxEraserSolventsGUI-0.8.4.jar*. On most systems, it is enough to double-click it. If you are not able to directly run it, open a command line window (like Command Prompt or PowerShell on Windows systems) move to the application folder and type:

java -jar ToxEraserSolventsGUI-0.8.4.jar

LINUX/MAC OS

- Make sure to install the latest LTS version of Java. First, in a shell update the apt package index with *sudo apt update* command.
- Once the package index is updated install the default Java OpenJDK package with *sudo apt install default-jdk*
- When the installation is complete, move to the application folder and execute *sh starter.sh* or *bash starter.sh*, or double click on *starter.sh* file

3. How to use

3.1 User Requirements Input

ToxEraser Solvents has a user-friendly graphical interface, in which the user adds the structure of interest, defines the similarity threshold and runs the calculation. The structure can be entered using a SMILES string.

3.1.1 Insert the solvent to substitute

In the main application window, the user can insert a single structure entering its SMILES (see figure 1). The software searches this structure in the internal archive of ingredients implemented within the software.

Figure 1: The figure shows how to add the solvent of interest

3.1.2 Insert the similarity threshold

In the GUI, the user has to select which similarity threshold wants to use to filter the substituents (see figure 2). This means that the software will show the substituents for which the similarity with the target is higher than the threshold set up by the end user. It is important to underline that the

software provides the substituents for each safety level class. The similarity algorithm used by the software is that calculated by VEGA (Floris et al., 2014).

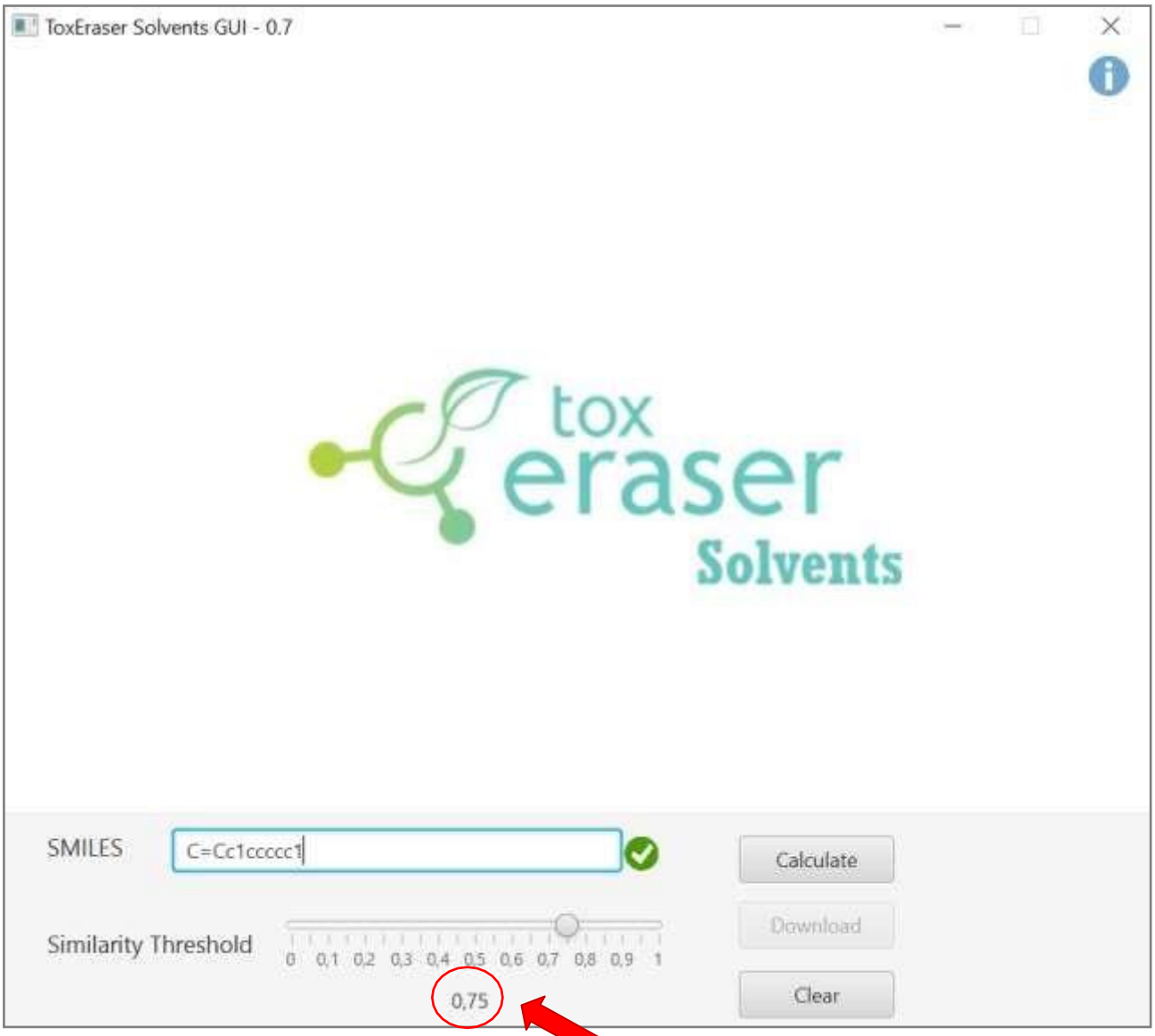

Figure 2: Selection of the similarity threshold

3.1.3 Run calculation

Once each parameter has been correctly set, the user has to click on the button **'Calculate'** in order to start the calculation (see figure 3).

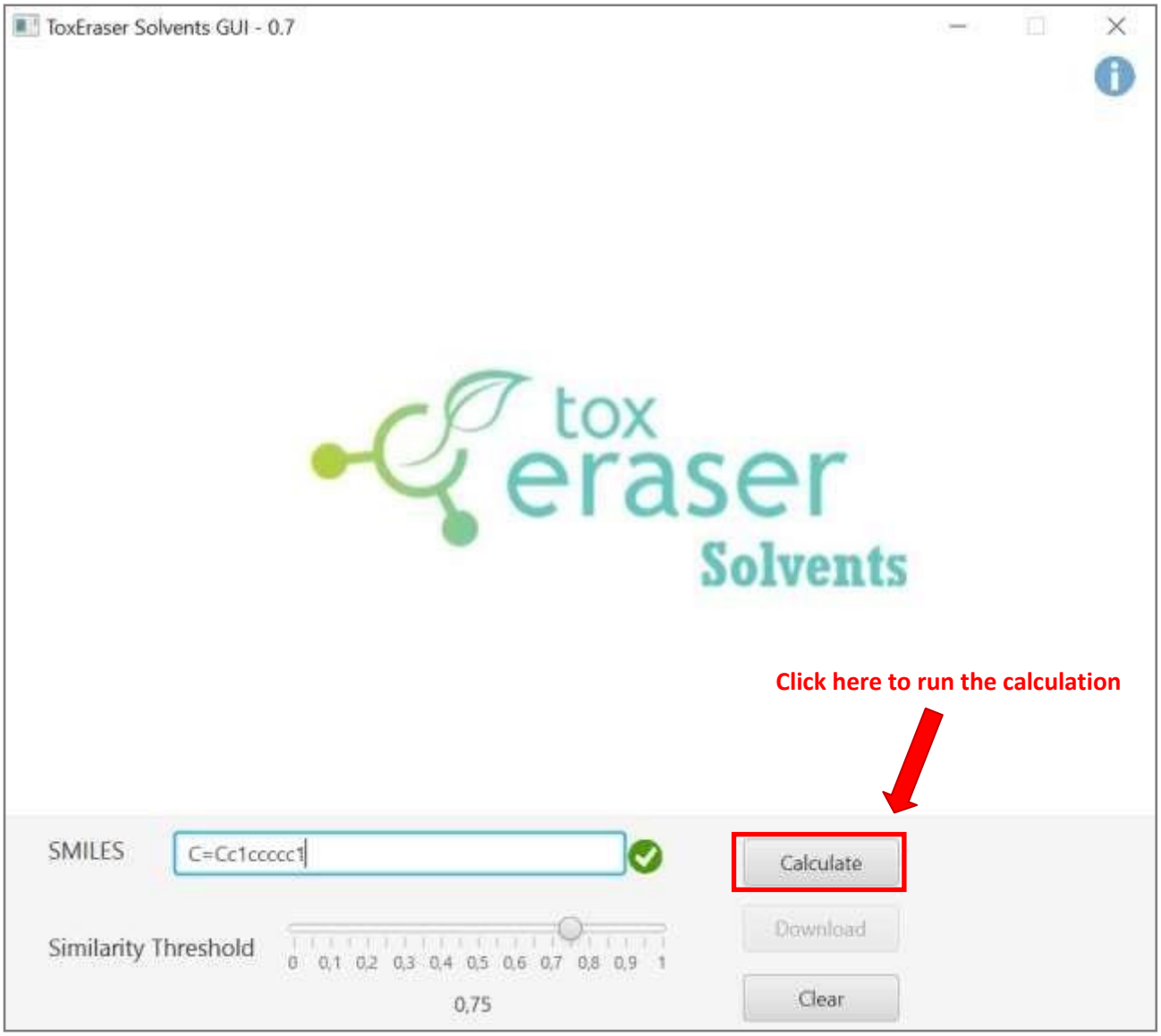

Figure 3: The figure shows how to start the calculation

3.1.4 Download the output and selection of the directory

Once the calculation is concluded, the software indicates that the output is ready to download (see figure 4). The user has to click the **'Download'** button to download the results (see figure 5). Then the user has to select the directory of the output; he/she has to select the folder, indicate a name and save the file (see figure 6). The output is a PDF file.

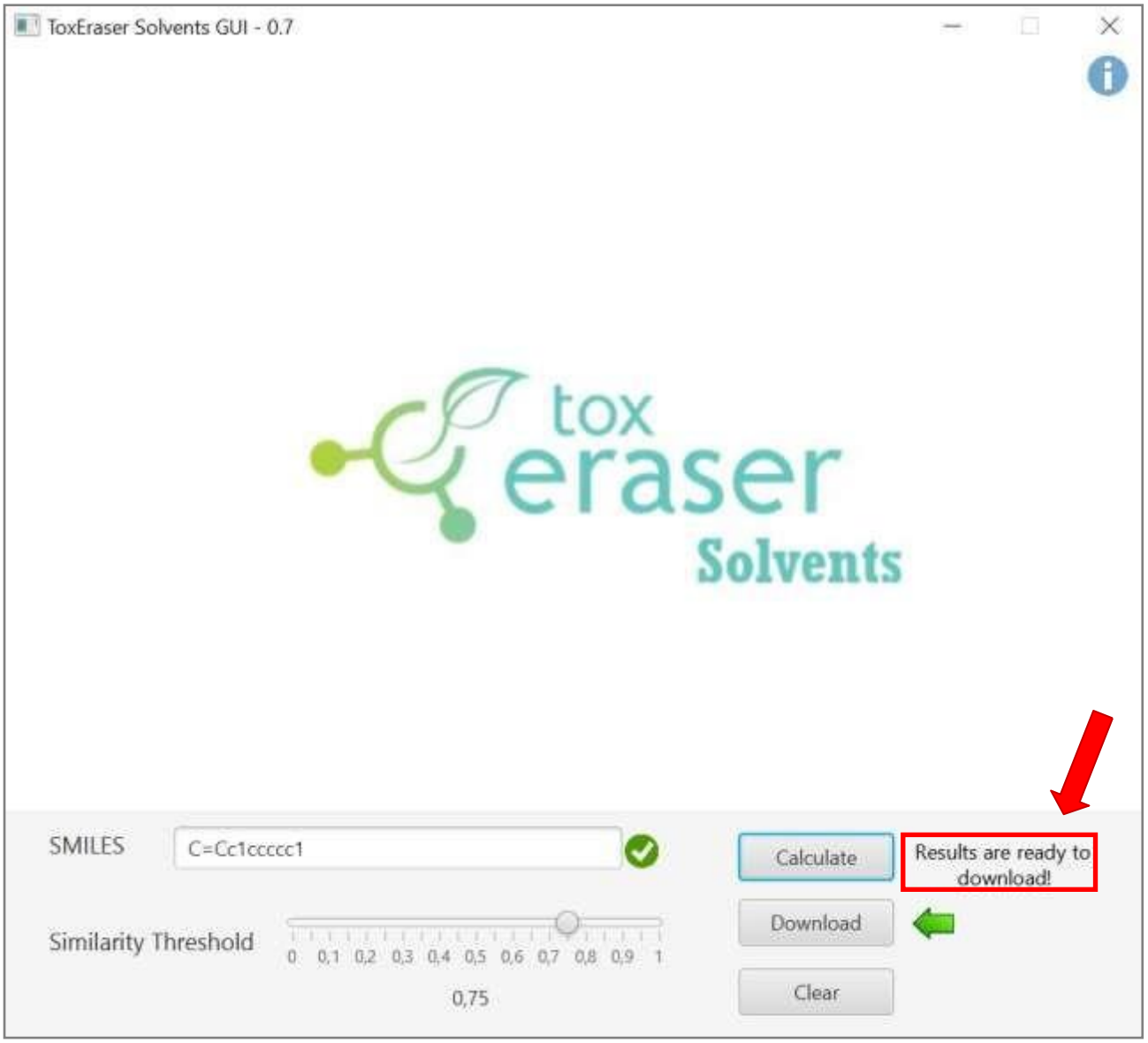

Figure 4: The software shows that results are ready to download.

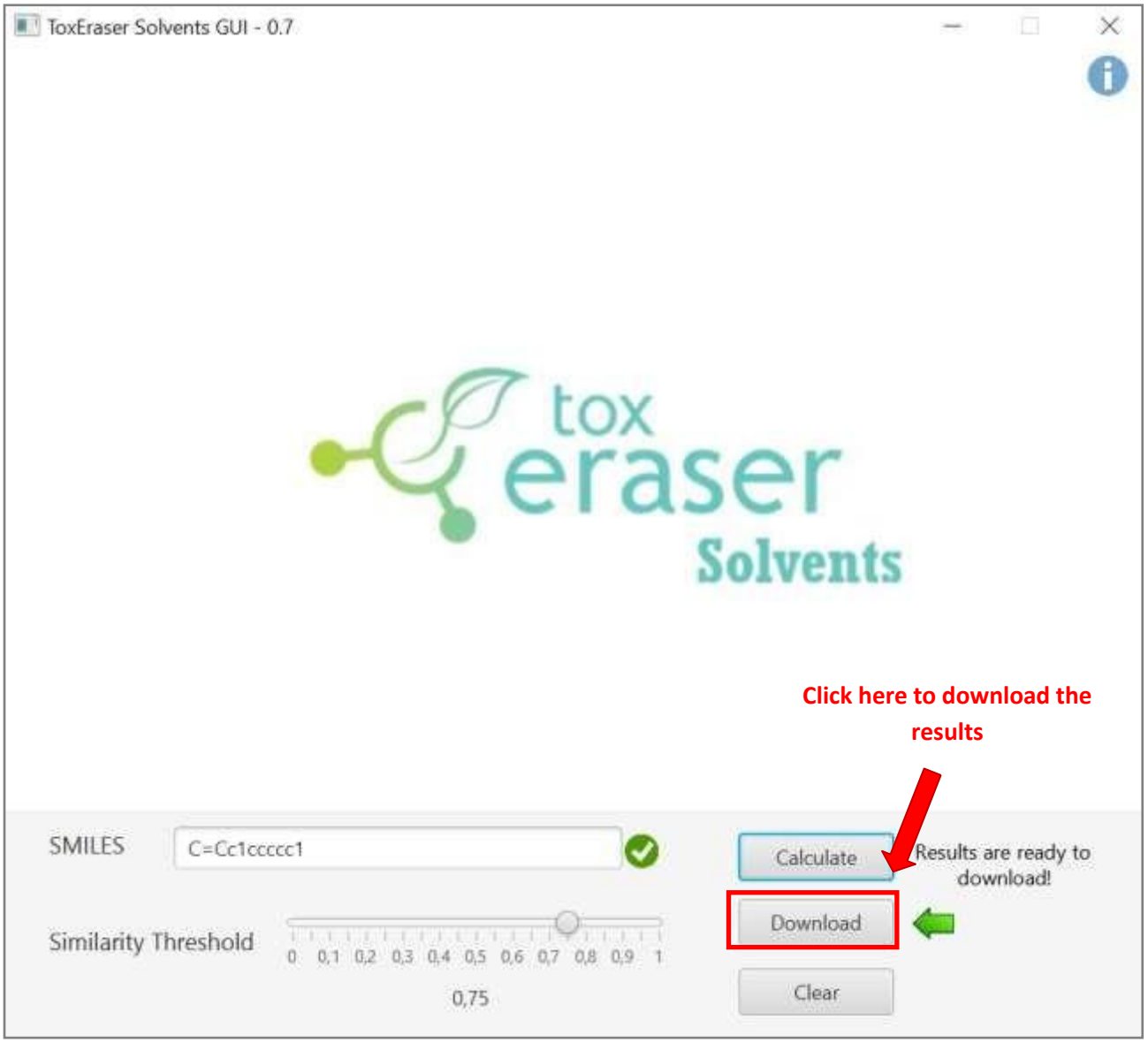

Figure 5: The figure shows how to download the results.

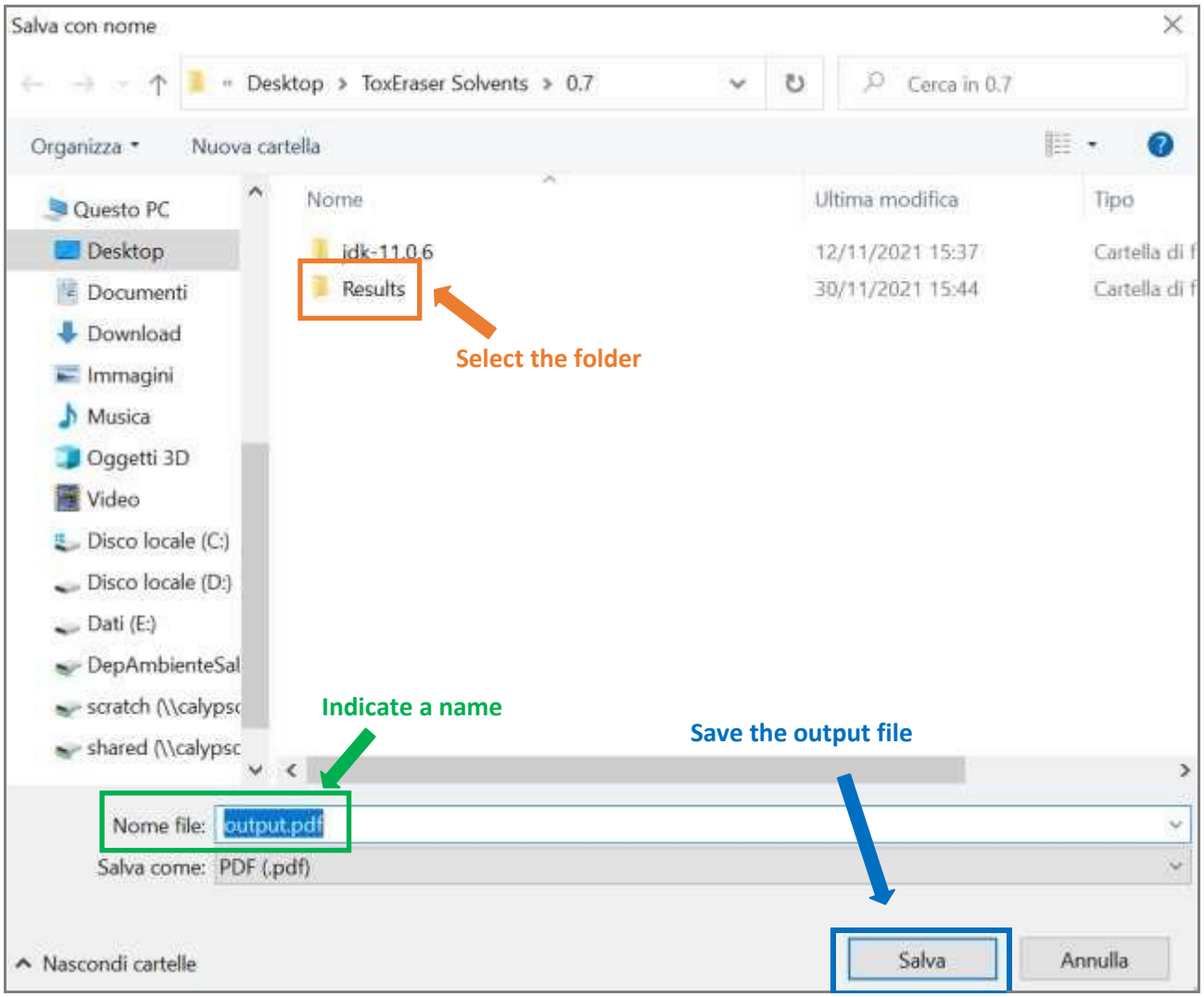

Figure 6: The figure shows how to select the output directory

3.2 Software elaboration

ToxEraser Solvents provides a PDF output file. In the first part of the report, the software provides (if found) a matching molecule from the archive, with all its details (see figure 7). If the molecule is not present in the database, no match will be possible.
Following, the list of safer compounds is reported.
The list is subdivided in four different sections showing the safer substituents of each safety class. An explanation of the four safety classes is provided in the Appendix II.
Found molecules are reported sorted from the most similar to the least similar, applying a read- across approach. The software will show only the substituents with a similarity index higher than the threshold chosen as minimum level.

A screenshot of the output is shown here (see figure 8), while a complete output generated by the software is shown in the Appendix III of this user guide.

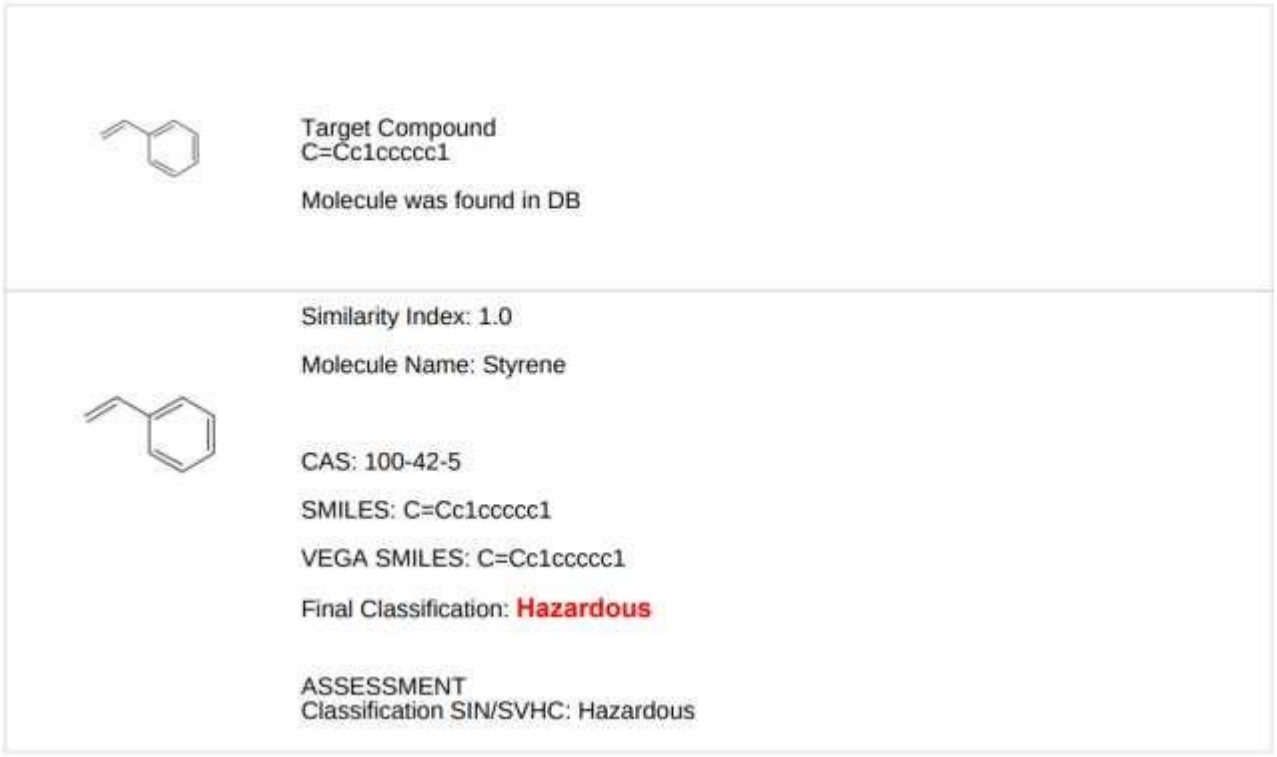

Figure 7: First part of the output. The software shows a possible matching molecule form the archive.

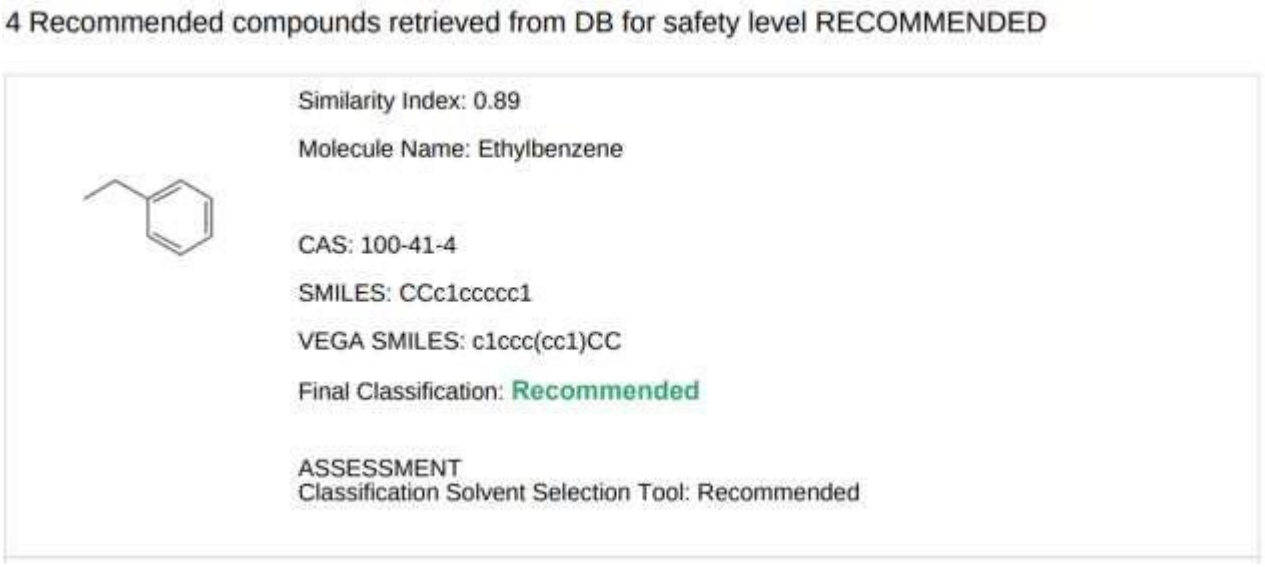

Figure 8: Screenshot of the output provided by ToxEraser Solvents (first recommended substituent of Styrene).

4. Acknowledgements and contacts

ToxEraser Solvents was developed within the LIFE project VERMEER [LIFE16 ENV/IT/000167] (https://www.life-vermeer.eu/). The project is coordinated by Istituto di Ricerche Farmacologiche Mario Negri IRCCS.
The partners of the project are: Electricitè de France (EDF), SCIENSANO, SC Sviluppo Chimica s.p.a., German Federal Institute for Risk Assessment (BfR), Angel Consulting SAS, Institute National de l'Environnement Industriel et des Risques (INERIS), AFRY.

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a.manganaro@kode-solutions.net
emilio.benfenati@marionegri.it

5. References

Floris, M., Manganaro, A., Nicolotti, O. *et al.* A generalizable definition of chemical similarity for read-across. *J Cheminform* 6, 39 (2014). https://doi.org/10.1186/s13321-014-0039-1

Prat, D., Wells, A., Hayler, J., Sneddon, H., McElroy, R.C., Abou-Shehada , S., and Dunn, P.J. CHEM21 selection guide of classical – and less classical- solvents. ***Green Chem.***, 2016,**18**, 288-296. https://doi.org/10.1039/C5GC01008J

Sels, H.; De Smet, H.; Geuens, J. SUSSOL—Using Artificial Intelligence for Greener Solvent Selection and Substitution. *Molecules* **2020**, *25*, 3037. https://doi.org/10.3390/molecules25133037

● APPENDIX I: lists used to generate the level of safety

ToxEraser Solvents uses five authoritative lists retrieved from publicly available databases and from literature. By exploiting the evidences provided by these lists, a global integrated assessment was developed assigning a final label for each safety level. This concept is described in detail in the Appendix II.

The lists used are:

- SUSSOL (Sustainable Solvents Selection and Substitution Software) tool list: this list is extracted from the work of Sels (Sels et al., 2020). In this paper the development of a tool for the solvents selection and substitution is described. For the implementation of this tool, authors decided to integrate the CHEM21 approach (Prat et al., 2015). This represents a robust and recognized approach. The CHEM21 methodology assigns scores for safety (S), health (H), and environment (E) criteria, aligned with the Global Harmonized System (GHS) and European regulations. Every criterion (SH&E) is assigned a score between 1 and 10, 10 representing the highest hazard in each category. A color code is associated with the scores: green for 1–3, yellow for 4–6, and red for 7–10. The combination of the three scores determines the final ranking of the solvent: hazardous (red), problematic (yellow), or recommended (green).
  The safety score is assigned based on the flash point and boiling point. Penalty points are assigned for a low auto ignition temperature, a high resistivity, or the ability to form peroxides. A solvent with a high energy of decomposition has a score of 10.
  The health score is determined by the compounds H3xx statements. More severe H3xx statements yield higher scores. A penalty point is added to the score for low boiling point (<85 °C) solvents. Solvents with incomplete toxicological data are assigned a score of 5.
  The score for environmental impact is based on the solvent's boiling point, the H4xx statements, and the REACH status. An ideal boiling range between 70 and 139 °C is proposed. Solvents with lower boiling points are more likely to give rise to emissions, but a high boiling solvent is more difficult to recycle. Solvents with incomplete environment toxicity data are assigned a score of 5. Solvents with the H420 statement (ozone layer hazard) have a score of 10 by default.
  The scores for SH&E and the corresponding color codes are self-explanatory and provide useful information to the user.
- SUSSOL Tool – free data: are data extracted from the same publication and they are provided to the user in the free version of the SUSSOL tool. We decided to consider this list in order to avoid losing information.
- Solvent Selection Tool list: The list is downloaded from the Solvents Selection Tool. This tool is freely provided by the ACS GCI Pharmaceutical Roundtable (GCIPR). It is an approximate duplicate of the original tool built by AstraZeneca, a proprietary technology, and later donated to the ACS GCIPR. More information about the tool can be found in the original open access work by Diorazio (Diorazio et al., 2016). An evaluation of Safety, Health and Environmental criteria is provided following the same approach previously described for the SUSSOL lists.

- Safer Chemical Ingredient List (SCIL): This list is designed to help manufacturers in finding safer alternatives that meet the criteria of the Safer Choice Program, concerning the evaluation of both experimental and modeled data. This program, sponsored by the United States Environmental Protection Agency (US EPA) was conceived to help stakeholders to find safer solutions for human health and the environment.
- SIN list: The list is a comprehensive list of substances that has been identified by *ChemSec* as fulfilling the criteria for Substances of Very High Concern (SVHC), as described in the EU REACH Regulation article 57.

● APPENDIX II: the safety level meta-concept

As described in the Appendix I, ToxEraser Solvents uses different lists retrieved from different publicly sources. The judgements provided by each list for each item were merged into a single global judgement, to obtain a final meta-classification where solvents can be found ordered according to a rank of safety. By applying this concept, four different safety level were proposed based on the global assessment of each item:

- Recommended, when the solvent is considered as Recommended by one or more lists
- Problematic, when solvent presents global evidence of problematic nature
- Hazardous, when lists are concordant to detect the solvent as hazardous
- Conflictual assessment, when lists present disagreement assessments

As described above, in the output report the safer compounds for each of these classes are displayed.

● APPENDIX III: example of a complete output file

A complete output is shown in this section to better express the structure of the file.

In this example, the following conditions are set up:

- Target molecule: Styrene (Hazardous)
- Similarity threshold: 0.60

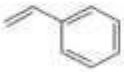
TOX ERASER SOLVENTS- REPORT

ANALYSIS RESULTS FOR TARGET MOLECULE C=Cc1ccccc1

TOX ERASER SOLVENTS - VERSION 0.7

Target Compound
C=Cc1ccccc1

Molecule was found in DB



Similarity Index: 1.0

Molecule Name: Styrene

CAS: 100-42-5

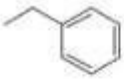
SMILES: C=Cc1ccccc1

VEGA SMILES: C=Cc1ccccc1

Final Classification: **Hazardous**

ASSESSMENT
Classification SIN/SVHC: Hazardous

4 Recommended compounds retrieved from DB for safety level RECOMMENDED



Similarity Index: 0.89

Molecule Name: Ethylbenzene

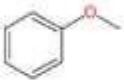
CAS: 100-41-4

SMILES: CCc1ccccc1

VEGA SMILES: c1ccc(cc1)CC

Final Classification: **Recommended**

ASSESSMENT
Classification Solvent Selection Tool: Recommended



Similarity Index: 0.73

Molecule Name: Anisole

CAS: 100-66-3

SMILES: COc1ccccc1

VEGA SMILES: O(c1ccccc1)C

Final Classification: **Recommended**

ASSESSMENT
Classification Solvent Selection Tool: Recommended
Classification SUSSOL Tool: Recommended
Classification SUSSOL Tool - free version: Recommended

Similarity Index: 0.62

Molecule Name: Thiophene

CAS: 01/31/10

SMILES: s1cccc1

VEGA SMILES: c1ccsc1

Final Classification: **Recommended**

ASSESSMENT
Classification Solvent Selection Tool: Recommended

Similarity Index: 0.61

Molecule Name: Pyrrole

CAS: 109-97-7

SMILES: [nH]1cccc1

VEGA SMILES: c1cc[nH]c1

Final Classification: **Recommended**

ASSESSMENT
Classification Solvent Selection Tool: Recommended

29 Problematic compounds retrieved from DB for safety level PROBLEMATIC

Similarity Index: 0.92

Molecule Name: Toluene

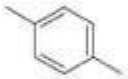
CAS: 108-88-3

SMILES: Cc1ccccc1

VEGA SMILES: c1ccc(cc1)C

Final Classification: Problematic

ASSESSMENT
Classification Solvent Selection Tool: Problematic
Classification SUSSOL Tool: Problematic
Classification SUSSOL Tool - free version: Problematic



Similarity Index: 0.89

Molecule Name: p-Xylene

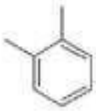
CAS: 106-42-3

SMILES: Cc1ccc(C)cc1

VEGA SMILES: c1cc(ccc1C)C

Final Classification: Problematic

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.89

Molecule Name: o-xylene

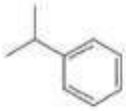
CAS: 95-47-6

SMILES: Cc1ccccc1C

VEGA SMILES: c1ccc(c(c1)C)C

Final Classification: Problematic

ASSESSMENT
Classification SUSSOL Tool: Problematic
Classification SUSSOL Tool - free version: Problematic



Similarity Index: 0.87

Molecule Name: Isopropylbenzene

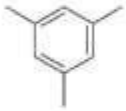
CAS: 98-82-8

SMILES: CC(C)c1ccccc1

VEGA SMILES: c1ccc(cc1)C(C)C

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.86

Molecule Name: Mesitylene [1,3,5-Trimethylbenzene]

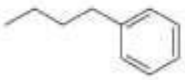
CAS: 108-67-8

SMILES: Cc1cc(C)cc(C)c1

VEGA SMILES: c1c(cc(cc1C)C)C

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.82

Molecule Name: Butylbenzene

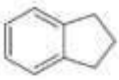
CAS: 104-51-8

SMILES: CCCCc1ccccc1

VEGA SMILES: c1ccc(cc1)CCCC

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.8

Molecule Name: Indane

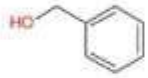
CAS: 11/06/96

SMILES: C1Cc2ccccc2C1

VEGA SMILES: c1ccc2c(c1)CCC2

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.79

Molecule Name: benzyl alcohol

CAS: 100-51-6

SMILES: OCc1ccccc1

VEGA SMILES: OCc1ccccc1

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic
Classification SUSSOL Tool: Problematic

Similarity Index: 0.78

Molecule Name: Tetralin

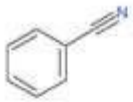
CAS: 119-64-2

SMILES: C1CCc2ccccc2C1

VEGA SMILES: c1ccc2c(c1)CCCC2

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.78

Molecule Name: Benzonitrile

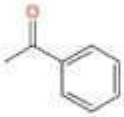
CAS: 100-47-0

SMILES: N#Cc1ccccc1

VEGA SMILES: N#Cc1ccccc1

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.78

Molecule Name: Acetophenone

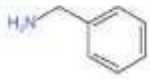
CAS: 98-86-2

SMILES: CC(=O)c1ccccc1

VEGA SMILES: O=C(c1ccccc1)C

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.77

Molecule Name: Benzylamine

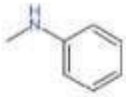
CAS: 100-46-9

SMILES: NCc1ccccc1

VEGA SMILES: NCc1ccccc1

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.72

Molecule Name: N-Methylaniline

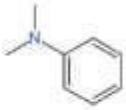
CAS: 100-61-8

SMILES: CNc1ccccc1

VEGA SMILES: c1ccc(cc1)NC

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.72

Molecule Name: N,N-Dimethylaniline

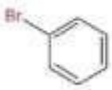
CAS: 121-69-7

SMILES: CN(C)c1ccccc1

VEGA SMILES: c1ccc(cc1)N(C)C

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.72

Molecule Name: Bromobenzene

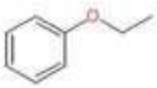
CAS: 108-86-1

SMILES: Brc1ccccc1

VEGA SMILES: c1ccc(cc1)Br

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.71

Molecule Name: Ethoxybenzene [phenetole]

CAS: 103-73-1

SMILES: CCOc1ccccc1

VEGA SMILES: O(c1ccccc1)CC

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic

Similarity Index: 0.71

Molecule Name: Chlorobenzene

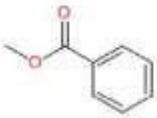
CAS: 108-90-7

SMILES: Clc1ccccc1

VEGA SMILES: c1ccc(cc1)Cl

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic
Classification SUSSOL Tool: Problematic



Similarity Index: 0.71

Molecule Name: Methyl benzoate

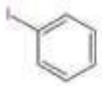
CAS: 93-58-3

SMILES: COC(=O)c1ccccc1

VEGA SMILES: O=C(OC)c1ccccc1

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.71

Molecule Name: Iodobenzene

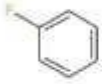
CAS: 591-50-4

SMILES: Ic1ccccc1

VEGA SMILES: c1ccc(cc1)I

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.71

Molecule Name: Fluorobenzene

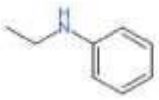
CAS: 462-06-6

SMILES: Fc1ccccc1

VEGA SMILES: Fc1ccccc1

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.71

Molecule Name: N-Ethylaniline

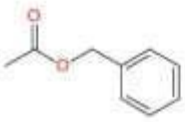
CAS: 103-69-5

SMILES: CCNc1ccccc1

VEGA SMILES: c1ccc(cc1)NCC

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.69

Molecule Name: Benzyl acetate

CAS: 140-11-4

SMILES: CC(=O)OCc1ccccc1

VEGA SMILES: O=C(OCc1ccccc1)C

Final Classification: **Problematic**

ASSESSMENT
Classification SUSSOL Tool: Problematic

Similarity Index: 0.68

Molecule Name: 2-Methylpyridine [2-Picoline]

CAS: 109-06-8

SMILES: Cc1ccccn1

VEGA SMILES: n1ccccc1C

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic

Similarity Index: 0.67

Molecule Name: Dibenzyl ether

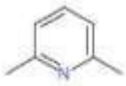
CAS: 103-50-4

SMILES: C(OCc1ccccc1)c2ccccc2

VEGA SMILES: O(Cc1ccccc1)Cc2ccccc2

Final Classification: **Problematic**

ASSESSMENT
Classification SUSSOL Tool: Problematic



Similarity Index: 0.67

Molecule Name: 2,6-Dimethylpyridine [2,6-Lutidine]

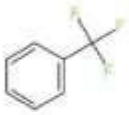
CAS: 108-48-5

SMILES: Cc1cccc(C)n1

VEGA SMILES: n1c(cccc1C)C

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.66

Molecule Name: Benzotrifluoride

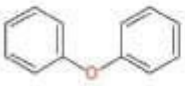
CAS: 98-08-8

SMILES: FC(F)(F)c1ccccc1

VEGA SMILES: FC(F)(F)c1ccccc1

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.65

Molecule Name: Diphenyl Ether

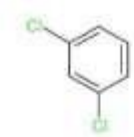
CAS: 101-84-8

SMILES: O(c1ccccc1)c2ccccc2

VEGA SMILES: O(c1ccccc1)c2ccccc2

Final Classification: **Problematic**

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.65

Molecule Name: 1,3-Dichlorobenzene

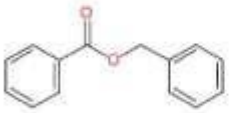
CAS: 541-73-1

SMILES: Clc1cccc(Cl)c1

VEGA SMILES: c1cc(cc(c1)Cl)Cl

Final Classification: Problematic

ASSESSMENT
Classification Solvent Selection Tool: Problematic



Similarity Index: 0.62

Molecule Name: Benzyl Benzoate

CAS: 120-51-4

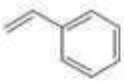
SMILES: O=C(OCc1ccccc1)c2ccccc2

VEGA SMILES: O=C(OCc1ccccc1)c2ccccc2

Final Classification: Problematic

ASSESSMENT
Classification Solvent Selection Tool: Problematic

14 Hazardous compounds retrieved from DB for safety level HAZARDOUS



Similarity Index: 1

Molecule Name: Styrene

CAS: 100-42-5

SMILES: C=Cc1ccccc1

VEGA SMILES: C=Cc1ccccc1

Final Classification: **Hazardous**

ASSESSMENT
Classification SIN/SVHC: Hazardous

Similarity Index: 0.85

Molecule Name: Benzene

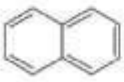
CAS: 71-43-2

SMILES: c1ccccc1

VEGA SMILES: c1ccccc1

Final Classification: **Hazardous**

ASSESSMENT
Classification Solvent Selection Tool: Highly Hazardous
Classification SUSSOL Tool: Hazardous
Classification SUSSOL Tool - free version: Hazardous
Classification SIN/SVHC: Hazardous



Similarity Index: 0.8

Molecule Name: Naphthalene

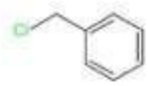
CAS: 91-20-3

SMILES: c1ccc2ccccc2c1

VEGA SMILES: c1ccc2ccccc2(c1)

Final Classification: **Hazardous**

ASSESSMENT
Classification SIN/SVHC: Hazardous



Similarity Index: 0.76

Molecule Name: Benzyl chloride

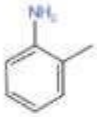
CAS: 100-44-7

SMILES: ClCc1ccccc1

VEGA SMILES: c1ccc(cc1)CCl

Final Classification: **Hazardous**

ASSESSMENT
Classification SIN/SVHC: Hazardous



Similarity Index: 0.76

Molecule Name: o-Toluidine

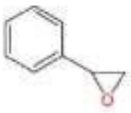
CAS: 95-53-4

SMILES: Cc1ccccc1N

VEGA SMILES: Nc1ccccc1C

Final Classification: **Hazardous**

ASSESSMENT
Classification SIN/SVHC: Hazardous



Similarity Index: 0.74

Molecule Name: Styrene oxide

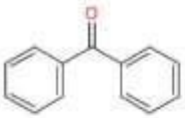
CAS: 96-09-3

SMILES: C1OC1c2ccccc2

VEGA SMILES: O1CC1c2ccccc2

Final Classification: **Hazardous**

ASSESSMENT
Classification SIN/SVHC: Hazardous



Similarity Index: 0.69

Molecule Name: Benzophenone

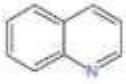
CAS: 119-61-9

SMILES: O=C(c1ccccc1)c2ccccc2

VEGA SMILES: O=C(c1ccccc1)c2ccccc2

Final Classification: **Hazardous**

ASSESSMENT
Classification SIN/SVHC: Hazardous



Similarity Index: 0.68

Molecule Name: Quinoline

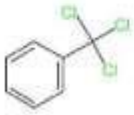
CAS: 91-22-5

SMILES: c1ccc2ncccc2c1

VEGA SMILES: n1cccc2ccccc12

Final Classification: **Hazardous**

ASSESSMENT
Classification Solvent Selection Tool: Hazardous
Classification SIN/SVHC: Hazardous



Similarity Index: 0.67

Molecule Name: Benzotrichloride

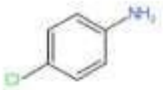
CAS: 98-07-7

SMILES: ClC(Cl)(Cl)c1ccccc1

VEGA SMILES: c1ccc(cc1)C(Cl)(Cl)Cl

Final Classification: **Hazardous**

ASSESSMENT
Classification SIN/SVHC: Hazardous



Similarity Index: 0.65

Molecule Name: 4-Chloroaniline

CAS: 106-47-8

SMILES: Nc1ccc(Cl)cc1

VEGA SMILES: Nc1ccc(cc1)Cl

Final Classification: **Hazardous**

ASSESSMENT
Classification SIN/SVHC: Hazardous

Similarity Index: 0.64

Molecule Name: Pyridine

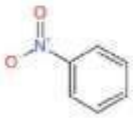
CAS: 110-86-1

SMILES: c1ccncc1

VEGA SMILES: n1ccccc1

Final Classification: **Hazardous**

ASSESSMENT
Classification Solvent Selection Tool: Hazardous
Classification SUSSOL Tool: Hazardous



Similarity Index: 0.63

Molecule Name: Nitrobenzene

CAS: 98-95-3

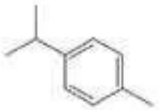
SMILES: [O-][N+](=O)c1ccccc1

VEGA SMILES: O=[N+]([O-])c1ccccc1

Final Classification: **Hazardous**

ASSESSMENT
Classification Solvent Selection Tool: Hazardous
Classification SIN/SVHC: Hazardous

3 Conflicting Assessment compounds retrieved from DB for safety level CONFLICTING ASSESSMENT



Similarity Index: 0.83

Molecule Name: p-cymene

CAS: 99-87-6

SMILES: CC(C)c1ccc(C)cc1

VEGA SMILES: c1cc(ccc1C)C(C)C

Final Classification: **Conflicting Assessment**

ASSESSMENT
Classification Solvent Selection Tool: Problematic
Classification SUSSOL Tool: Recommended
Classification SUSSOL Tool - free version: Recommended

Similarity Index: 0.73

Molecule Name: Aniline

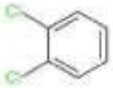
CAS: 62-53-3

SMILES: Nc1ccccc1

VEGA SMILES: Nc1ccccc1

Final Classification: **Conflicting Assessment**

ASSESSMENT
Classification Solvent Selection Tool: Problematic
Classification SIN/SVHC: Hazardous



Similarity Index: 0.65

Molecule Name: 1,2-Dichlorobenzene

CAS: 95-50-1

SMILES: Clc1ccccc1Cl

VEGA SMILES: c1ccc(c(c1)Cl)Cl

Final Classification: **Conflicting Assessment**

ASSESSMENT
Classification Solvent Selection Tool: Problematic
Classification SIN/SVHC: Hazardous