VERSION 0.8.6

USER GUIDE

Table of contents

1. Introduction

ToxEraser Cosmetics is a software designed for the cosmetic sector with the aim to identify risky substances and suggest safer alternatives as remedy. The approach applied for the substitution takes into account four main parameters: the level of safety, the functional uses, the similarity algorithm and the identification of hazardous functional groups/alerts. To determine the level of safety, the risk assessment addressed by seven Regulatory and other specialized European-US authoritative lists has been taken into account and the safety class emerging from the systematic evaluation and integration of each authority assessment was adopted. Details on the lists used in this work are reported in Appendix I, while the procedure applied to develop the safety level meta-concept is reported in Appendix II of this user guide. Then, we developed a hierarchical ontology of functions to enforce and facilitate the substitution process. Each ingredient is associated to one or more functional uses. Then, a read-across analysis enforces the substitution process making the substitution possible even when the ingredient is not included in the archive. An approach that incorporates together the level of safety, functions and similarity in a high-throughput way, would allow to easily recognize potential functional substitutes meeting the safety and the similarity criteria for a further and deeper evaluation. Finally, a series of structural alerts have been implemented in order to detect possible evidences 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 the skin sensitization ruleset implemented as in the Toxtree software.

ToxEraser Cosmetics works with a single ingredient, entered by the end user in the Graphical User Interface (GUI). ToxEraser Cosmetics 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).

The tool is designed to be joined with VERMEER Cosmolife (Selvestrel et al, 2021), in order to obtain a unique integrated powerful platform. Actually, the outcomes provided by ToxEraser, in its standalone architecture, can be deemed valuable to the extent they refer to substances collected in the ToxEraser list of cosmetic ingredients. Therein, ingredients are classified according to their safety on the ground of a systematic assessment performed by EU and US authoritative institutions. However, whenever a substance of interest is not included in the ToxEraser list, its substitution with safer molecule should be prompted by toxicological concerns, which cannot be dealt within the ToxEraser platform alone. Although the similarity metric could support the substitution of a molecule that is remarkably similar to unsafe molecules included in the list, further assessments are needed when this is not the case. That is right there that VERMEER Cosmolife gets into play, by yielding the level of risk of any molecule of interest. The scientific background of VERMEER Cosmolife can be found in its full detail in both the paper (Selvestrel et al., 2021) and dedicated websites (https://www.vegahub.eu/portfolio-item/toxeraser-cosmetics/) (https://www.life-vermeer.eu/download-software/software-toxeraser-cosmetics/).

2. Installing and starting ToxEraser Cosmetics

ToxEraser Cosmetics 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 Cosmetics 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 *ToxEraserGUI-0.8.6.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 ToxEraserGUI-0.8.6.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 Cosmetics has a user-friendly graphical interface, in which the user adds the structure and the functional use of interest, defines the similarity threshold and runs the calculation. The structure can be entered using a SMILES string.

3.1.1 Insert the ingredient 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.

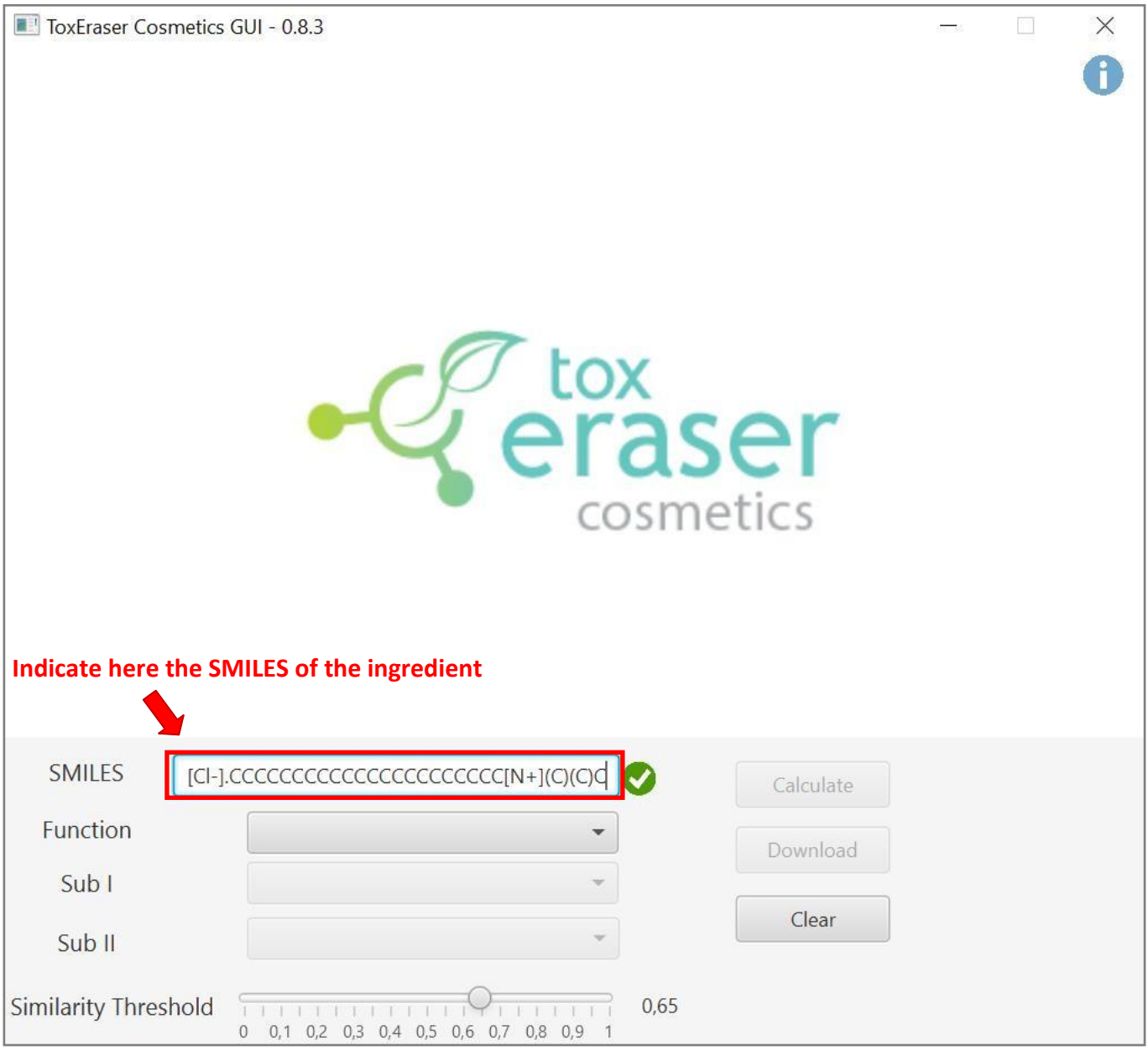


Figure 1: The figure shows how to add the ingredient of interest

3.1.2 Insert the functional use

In the GUI, the user has to insert the functional use of the ingredient. The software elaborates this input parameter providing as output only the safer substituents labelled with this specific functional category. Since the software contains a hierarchical ontology of functions, these last are organized on three levels of details and, in the drop-down menu, the user shall set the main function (see figure 2) or has the possibility to select the subcategories of the main function (see figure 3), or just leave the main function without any further specification. In this way, if only the main function is set up, the software provides a list of substituents belonging to this main category, while if also the subcategory is selected, the software provides a list of substituents belonging to this specific subcategory.

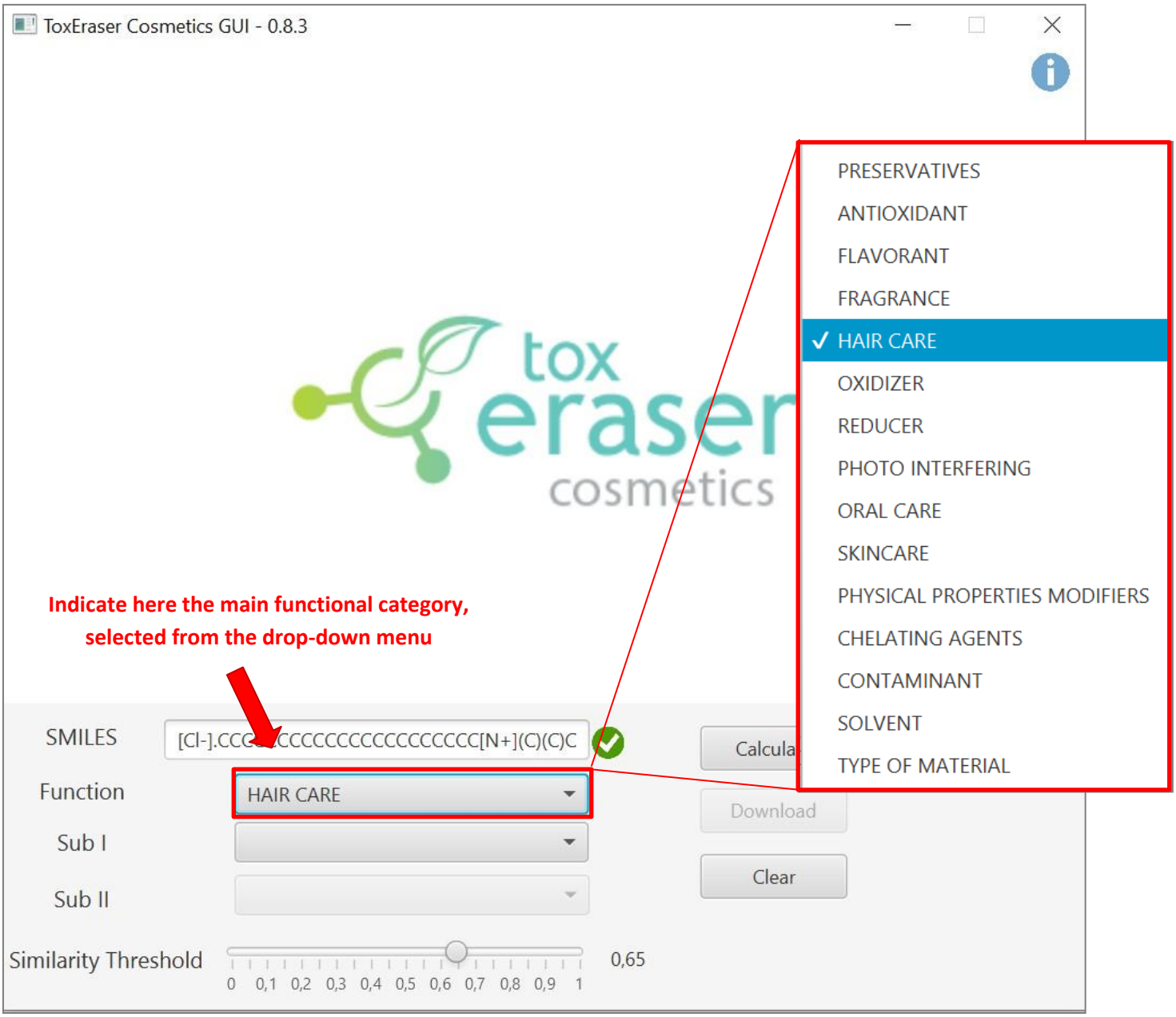


Figure 2: Selection of the main function

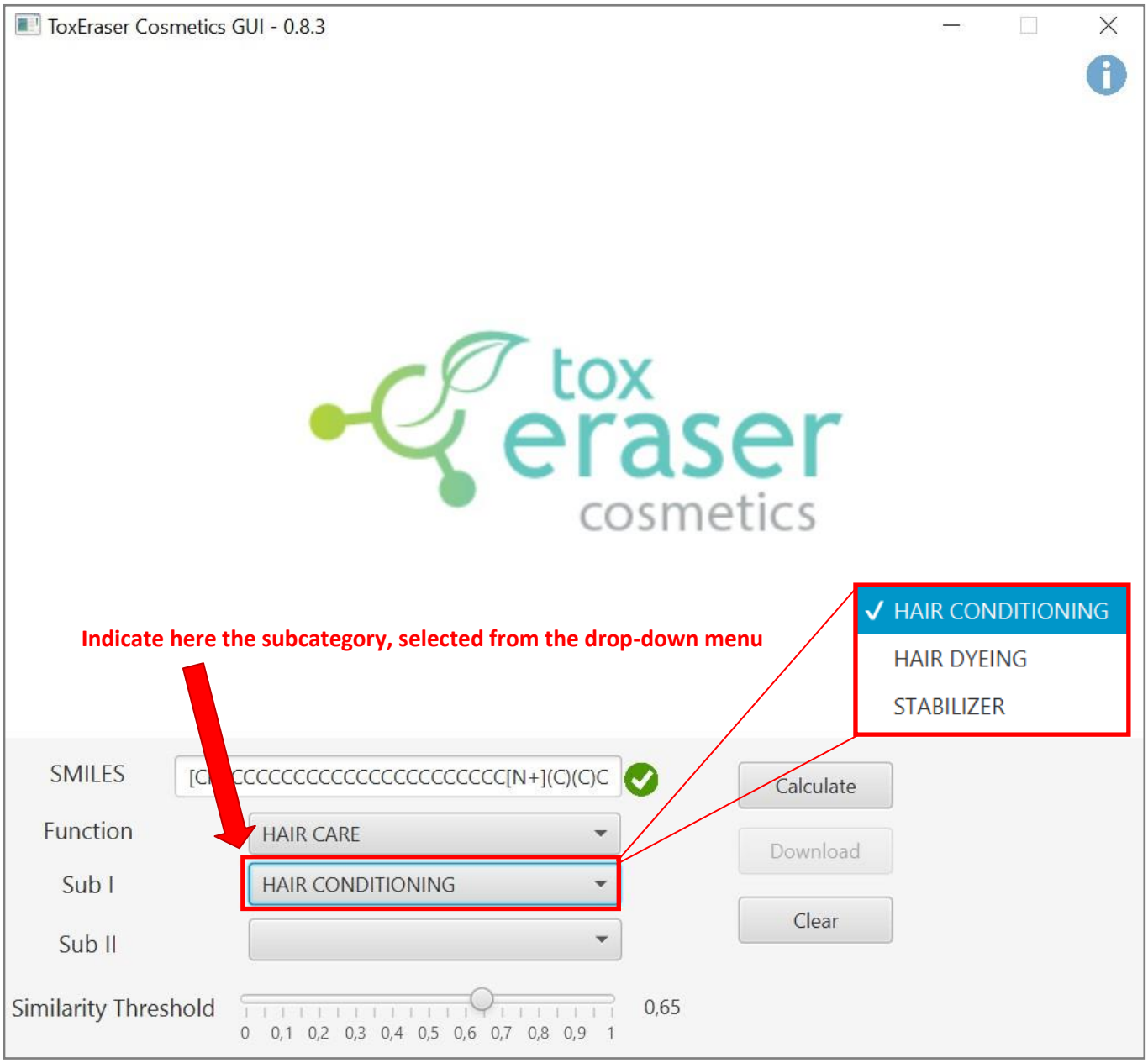


Figure 3: Selection of the subcategory

3.1.3 Insert the similarity threshold

In the GUI, the user has to select which similarity threshold wants to use to filter the substituents (see figure 4). 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).

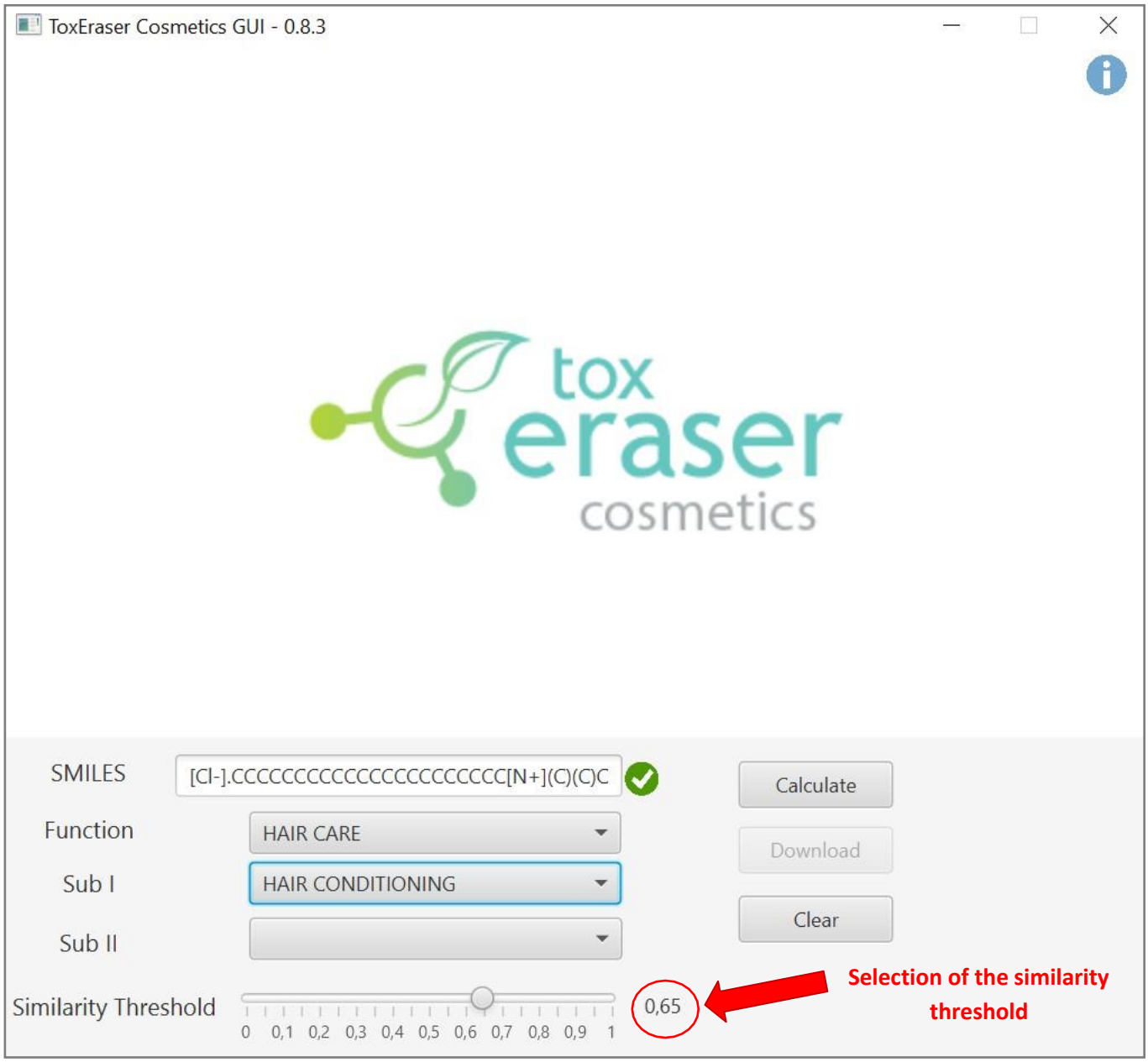


Figure 4: Selection of the similarity threshold

3.1.4 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 5).

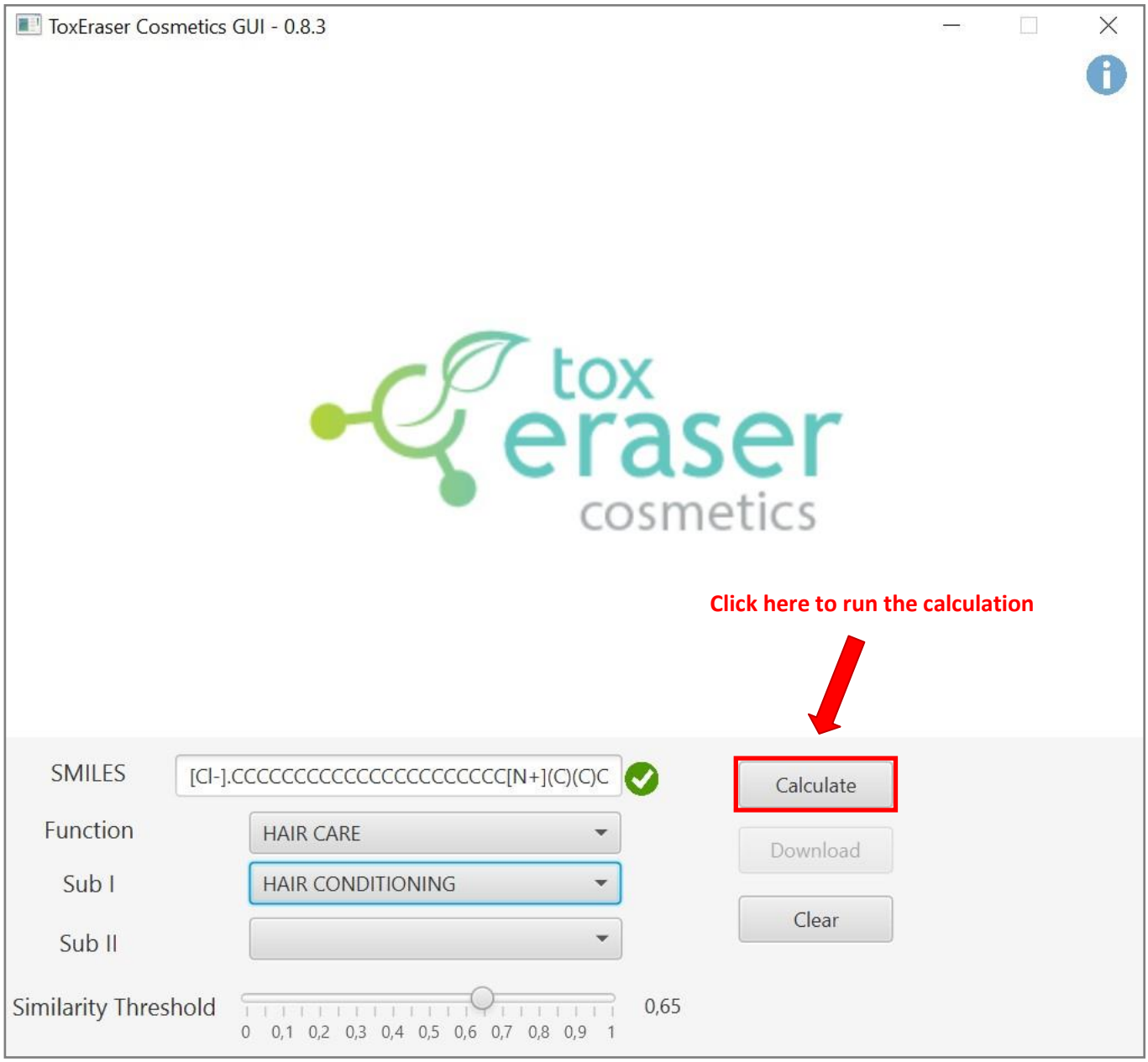


Figure 5: The figure shows how to start the calculation

3.1.5 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 6). The user has to click the **'Download'** button to download the results (see figure 7). 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 8). The output file is a PDF file.

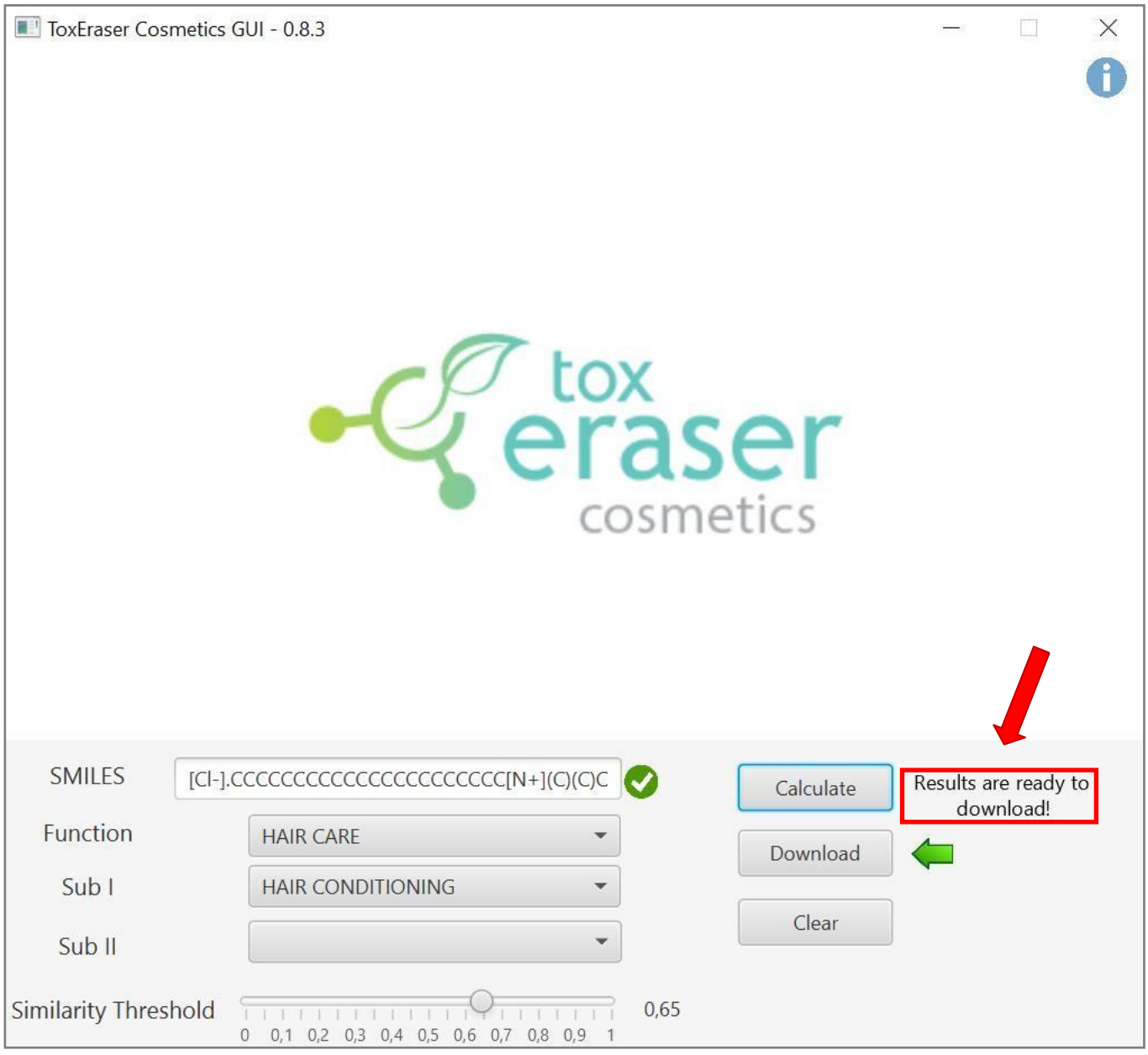


Figure 6: The software shows that results are ready to download.

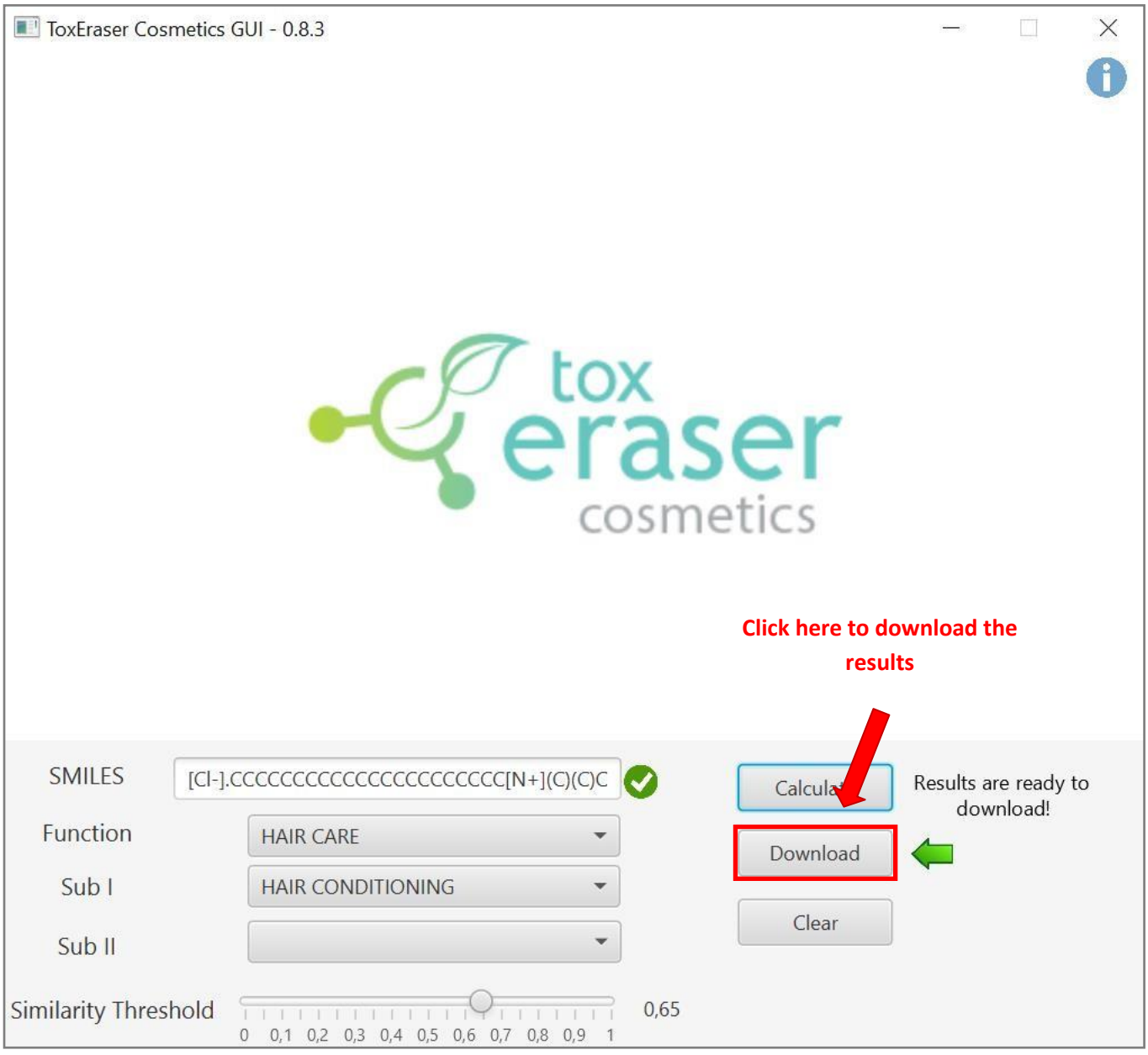


Figure 7: The figure shows how to download the results.

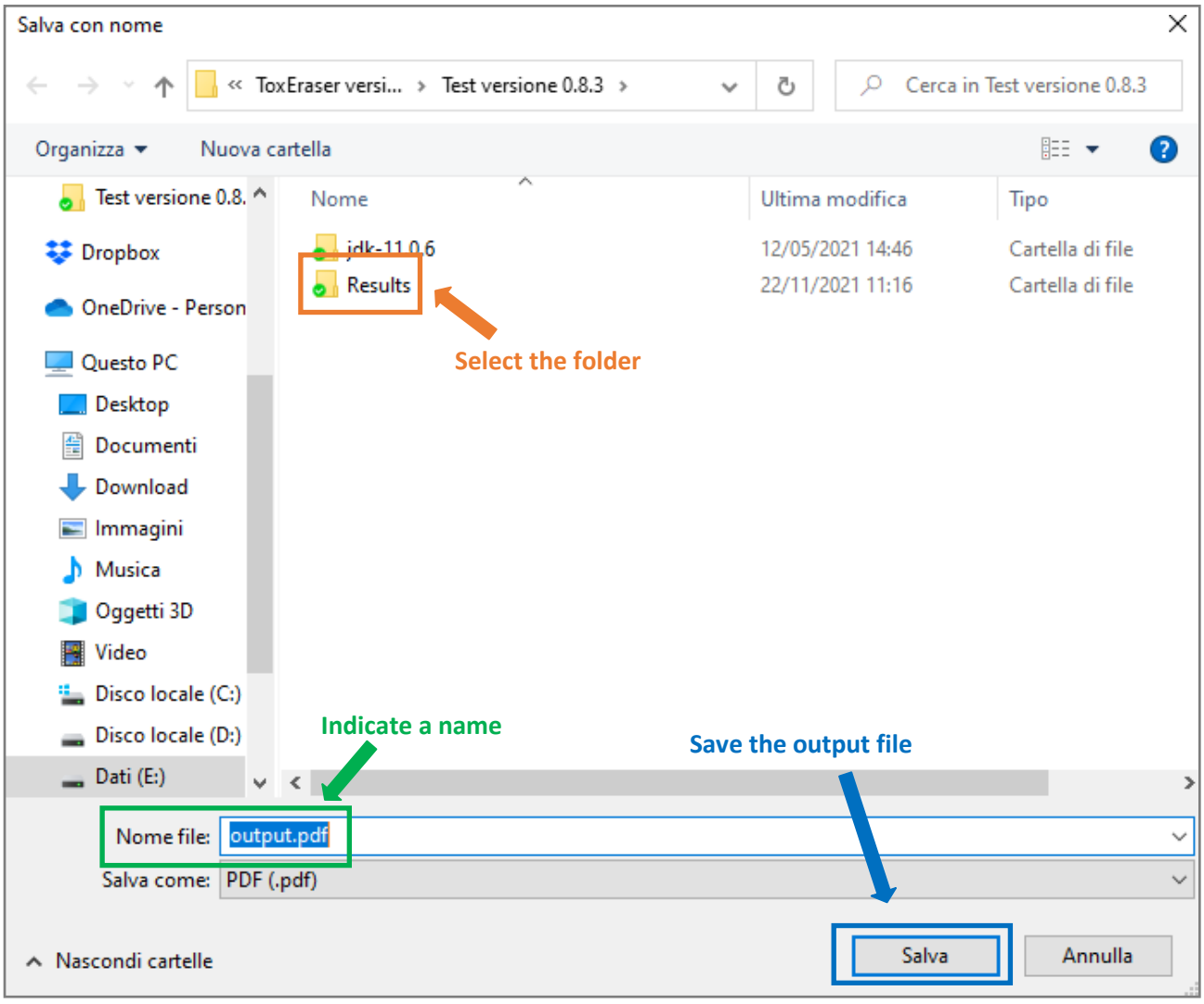


Figure 8: The figure shows how to select the output directory

3.2 Software elaboration

ToxEraser Cosmetics 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 9). The molecule is searched regardless of the user provided cosmetic function. If the molecule is not present in the database, no match will be possible.

Following, the list of compounds found with the same provided cosmetic function is reported.

The list is subdivided in five different sections showing the safer substituents of each safety class. An explanation of the five 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 10), while a complete output generated by the software is shown in the Appendix III of this user guide.

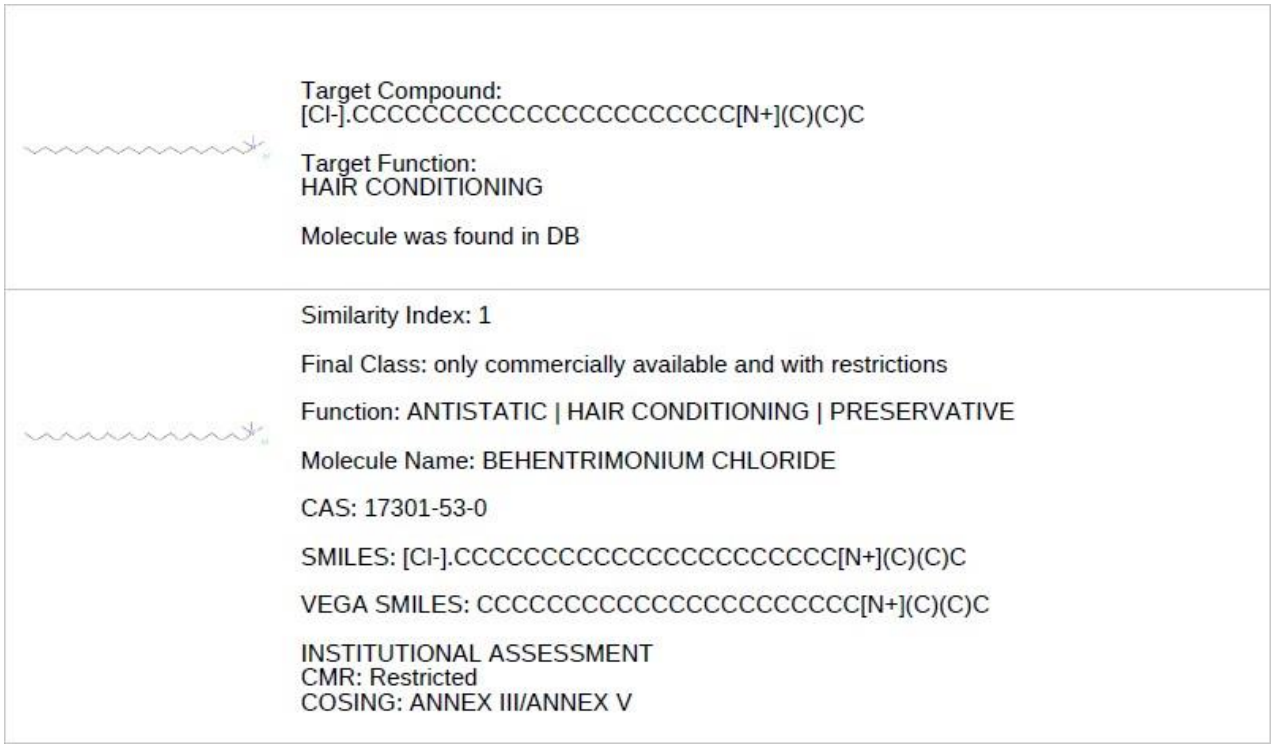


Figure 9: First part of the output. The software shows a possible matching molecule form the archive.

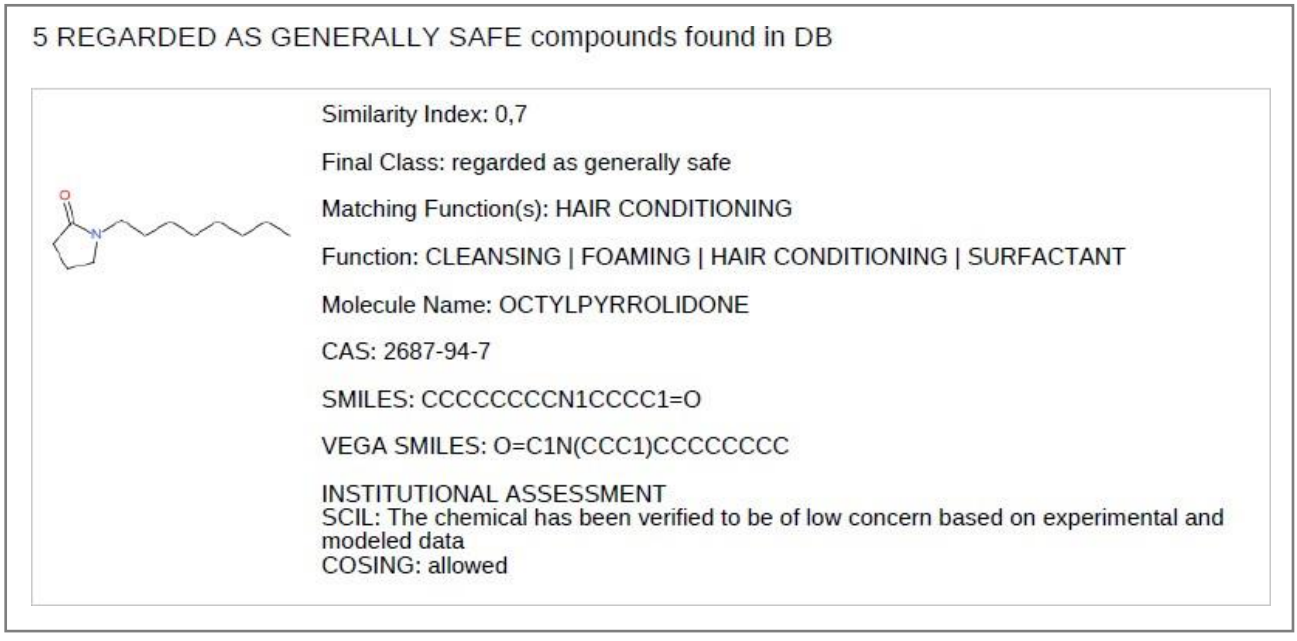


Figure 10: Screenshot of the output provided by ToxEraser (first substituent of Behentrimonium chloride considering hair conditioning as function).

4. Acknowledgements and contacts

ToxEraser Cosmetics 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.

For questions regarding the software and its use please contact:
gianluca.selvestrel@marionegri.it
davide.luciani@marionegri.it
a.manganaro@kode-solutions.net
emilio.benfenati@marionegri.it

5. References

EC - European Commission (2009). Regulation (EC) No 1223/2009 of the European Parliament and of the Council of 30 November 2009 on cosmetic products. Official Journal of European Union. L, 342, 59-209. http://data.europa.eu/eli/reg/2009/1223/2020-05-01

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

Selvestrel, G., Robino, F., Baderna, D., Manganelli, S., Asturiol, D., Manganaro, A., Zanotti Russo, M., Lavado, G., Toma, C., Roncaglioni, A. and Benfenati, E. (2021) "SpheraCosmolife: a new tool for the risk assessment of cosmetic products", *ALTEX - Alternatives to animal experimentation*. https://doi.org/10.14573/altex.2010221

APPENDIX I: lists used to generate the level of safety

ToxEraser Cosmetics uses seven authoritative lists drafted by different authorities, committees and regulatory agencies from Europe and USA. Each list contains ingredients thoughtfully evaluated by panel of experts considering several toxicological and ecotoxicological endpoints. 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:

- CosIng database: is the European Commission Database for information of cosmetic substances and ingredients and it is freely accessible on http://www.ec.europa.eu/growth/tools-databases/cosing/. CosIng contains information on the common ingredients allowed in cosmetic products and on the ingredients listed within the Annexes of the Cosmetic Regulation (EC) No. 1223/2009 (EC, 2009).
- 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.
- The Cosmetic Ingredient Review (CIR) is a company founded in the 1976 by the industry's trade association with the support of the U.S. Food and Drug Administration (FDA). The archive results from an extensive search of the world literature as part of its preparation for a safety assessment. Ingredients regarded as safe and safe with qualification were retrieved from this list.
- GRAS (Generally Recognize as Safe) list: A GRAS ingredient is an ingredient that has undergone safety evaluations by experts and has been proven not to cause harm when used as intended. General recognition of safety through scientific procedures is based upon the application of generally available and accepted scientific data, information, or methods.
- IFRA (International Fragrance Association) list: the IFRA developed a system to manage the safe use of fragrance materials. This system, the IFRA Standards, form the basis of the risk management strategy for the safe use of fragrance materials. The Expert Panel for Fragrance Safety reviews the activities of the Research Institute for Fragrance Materials (RIFM), and carries out a comprehensive risk assessment considering available information on several endpoints, determining the safety of fragrances. The assessment process asserts whether the ingredient should be (i) prohibited; (ii) restricted by a quantitative limit (iii) admitted under specific conditions.
- 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.
- CMR list: a list of Cancerogenic, Mutagenic or Reprotoxic (CMR) compounds extracted from the CosIng database.

APPENDIX II: the safety level meta-concept

As described in the Appendix I, ToxEraser uses seven authoritative lists drafted by different authorities and regulatory agencies. The judgements provided by each Institution for each item were merged into a single global judgement, to obtain a final meta-classification where cosmetic ingredients can be found ordered according to a rank of safety. For our purpose, in the safety ranking we took into account if the assessment is provided by both European and US institution or only the European ones. By applying this concept, only

ingredients regarded as safe without restrictions in both UE and US were treated as 'generally safe'. Concerning substances regarded as safe, both in UE and US, but supposed to have their use restricted, they can be found in the next category in terms of safety. Then we find the 'only commercially available' class, which includes ingredients which are allowed in the European market without any restrictions. Next, we found substances restricted in their use but not contemplated as safe in US lists, which are followed by the last category including either banned substances because reported in ANNEX II, or substances referred as prohibited in other lists.

To summarize, the five safety classes are:

- regarded as generally safe
- regarded as generally safe with restrictions
- only commercially available
- only commercially available with restrictions
- banned or not recommended

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:

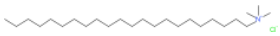
- Target molecule: Behentrimonium chloride
- Main function: Hair Care
- Subcategory 1: Hair conditioning
- Similarity threshold: 0.65

TOX ERASER COSMETICS - REPORT

ANALYSIS RESULTS FOR TARGET MOLECULE [Cl-].CCCCCCCCCCCCCCCCCCCCCC[N+](C)(C)C

TARGET FUNCTION: HAIR CONDITIONING

TOX ERASER COSMETICS VERSION - 0.8.3



Target Compound:
[Cl-].CCCCCCCCCCCCCCCCCCCCCC[N+](C)(C)C

Target Function:
HAIR CONDITIONING

Molecule was found in DB

Similarity Index: 1

Final Class: only commercially available and with restrictions

Function: ANTISTATIC | HAIR CONDITIONING | PRESERVATIVE

Molecule Name: BEHENTRIMONIUM CHLORIDE

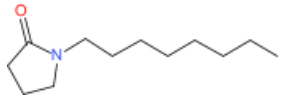
CAS: 17301-53-0

SMILES: [Cl-].CCCCCCCCCCCCCCCCCCCCCC[N+](C)(C)C

VEGA SMILES: CCCCCCCCCCCCCCCCCCCCCC[N+](C)(C)C

INSTITUTIONAL ASSESSMENT
CMR: Restricted
COSING: ANNEX III/ANNEX V

2 REGARDED AS GENERALLY SAFE compounds found in DB



Similarity Index: 0,7

Final Class: regarded as generally safe

Matching Function(s): HAIR CONDITIONING

Function: CLEANSING | FOAMING | HAIR CONDITIONING | SURFACTANT

Molecule Name: OCTYLPYRROLIDONE

CAS: 2687-94-7

SMILES: CCCCCCCCN1CCCC1=O

VEGA SMILES: O=C1N(CCC1)CCCCCCCC

INSTITUTIONAL ASSESSMENT
SCIL: The chemical has been verified to be of low concern based on experimental and modeled data
COSING: allowed

Similarity Index: 0,69

Final Class: regarded as generally safe

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | HAIR CONDITIONING

Molecule Name: DISTEAROYLETHYL DIMONIUM CHLORIDE

CAS: 67846-68-8

SMILES: [Cl-].CCCCCCCCCCCCCCCCCC(=O)OCC[N+](C)(C)CCOC(=O)CCCCCCCCCCCCCCCCCC

VEGA SMILES: O=C(OCC[N+](C)(C)CCOC(=O)CCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCC

INSTITUTIONAL ASSESSMENT
SCIL: The chemical has been verified to be of low concern based on experimental and modeled data
COSING: allowed

8 REGARDED AS GENERALLY SAFE WITH RESTRICTIONS compounds found in DB

Similarity Index: 0,93

Final Class: regarded as generally safe with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | HAIR CONDITIONING | PRESERVATIVE

Molecule Name: STEARTRIMONIUM BROMIDE

CAS: 1120-02-1

SMILES: [Br-].CCCCCCCCCCCCCCCCCC[N+](C)(C)C

VEGA SMILES: CCCCCCCCCCCCCCCCCC[N+](C)(C)C

INSTITUTIONAL ASSESSMENT
CIR: Safe with Qualifications
COSING: ANNEX V

Similarity Index: 0,88

Final Class: regarded as generally safe with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | EMULSIFYING | HAIR CONDITIONING

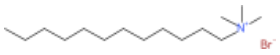
Molecule Name: DIMETHYL STEARAMINE

CAS: 124-28-7

SMILES: CCCCCCCCCCCCCCCCCCN(C)C

VEGA SMILES: N(C)(C)CCCCCCCCCCCCCCCCCC

INSTITUTIONAL ASSESSMENT
CIR: Safe as used
COSING: ANNEX III



Similarity Index: 0,86

Final Class: regarded as generally safe with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | HAIR CONDITIONING | PRESERVATIVE

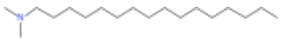
Molecule Name: LAURTRIMONIUM BROMIDE

CAS: 1119-94-4

SMILES: [Br-].CCCCCCCCCCCC[N+](C)(C)C

VEGA SMILES: CCCCCCCCCCCC[N+](C)(C)C

INSTITUTIONAL ASSESSMENT
CIR: Safe with Qualifications
COSING: ANNEX V



Similarity Index: 0,85

Final Class: regarded as generally safe with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | EMULSIFYING | HAIR CONDITIONING

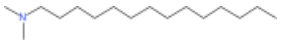
Molecule Name: DIMETHYL PALMITAMINE

CAS: 112-69-6

SMILES: CCCCCCCCCCCCCCCCN(C)C

VEGA SMILES: N(C)(C)CCCCCCCCCCCCCCCC

INSTITUTIONAL ASSESSMENT
CIR: Safe as used
COSING: ANNEX III



Similarity Index: 0,83

Final Class: regarded as generally safe with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | HAIR CONDITIONING

Molecule Name: DIMETHYL MYRISTAMINE

CAS: 112-75-4

SMILES: CCCCCCCCCCCCCCN(C)C

VEGA SMILES: N(C)(C)CCCCCCCCCCCCCC

INSTITUTIONAL ASSESSMENT
CIR: Safe as used
COSING: ANNEX III

Similarity Index: 0,8

Final Class: regarded as generally safe with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | HAIR CONDITIONING

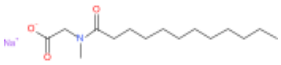
Molecule Name: DIMETHYL LAURAMINE

CAS: 112-18-5 | 52622-54-5

SMILES: CCCCCCCCCCCCN(C)C

VEGA SMILES: N(C)(C)CCCCCCCCCCCC

INSTITUTIONAL ASSESSMENT
CIR: Safe as used
COSING: ANNEX III



Similarity Index: 0,77

Final Class: regarded as generally safe with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | CLEANSING | EMULSIFYING | FOAMING | HAIR CONDITIONING | SKIN CONDITIONING | SURFACTANT | VISCOSITY CONTROLLING

Molecule Name: SODIUM LAUROYL SARCOSINATE

CAS: 137-16-6

SMILES: CCCCCCCCCCCC(=O)N(C)CC(=O)[O-].[Na+]

VEGA SMILES: O=C(O)CN(C(=O)CCCCCCCCCCC)C

INSTITUTIONAL ASSESSMENT
SCIL: The chemical has been verified to be of low concern based on experimental and modeled data
CIR: Safe with Qualifications
COSING: allowed

Similarity Index: 0,69

Final Class: regarded as generally safe with restrictions

Matching Function(s): HAIR CONDITIONING

Function: BINDING | EMULSIFYING | HAIR CONDITIONING | OPACIFYING | SKIN CONDITIONING | STABILISING

Molecule Name: STEARYL PALMITATE

CAS: 2598-99-4 | 100231-75-2

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCCCCCCC

VEGA SMILES: O=C(OCCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCC

INSTITUTIONAL ASSESSMENT
CIR: Safe with Qualifications
COSING: allowed

No ONLY COMMERCIALLY AVAILABLE AND WITHOUT RESTRICTIONS compounds found in DB

11 ONLY COMMERCIALLY AVAILABLE AND WITH RESTRICTIONS compounds found in DB

Similarity Index: 1

Final Class: only commercially available and with restrictions

Matching Function(s):

Function: ANTISTATIC | HAIR CONDITIONING | PRESERVATIVE

Molecule Name: BEHENTRIMONIUM CHLORIDE

CAS: 17301-53-0

SMILES: [Cl-].CCCCCCCCCCCCCCCCCCCCCC[N+](C)(C)C

VEGA SMILES: CCCCCCCCCCCCCCCCCCCCCC[N+](C)(C)C

INSTITUTIONAL ASSESSMENT
CMR: Restricted
COSING: ANNEX III/ANNEX V

Similarity Index: 0,92

Final Class: only commercially available and with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | HAIR CONDITIONING

Molecule Name: DIMETHYL BEHENAMINE

CAS: 21542-96-1

SMILES: CCCCCCCCCCCCCCCCCCCCCCN(C)C

VEGA SMILES: N(C)(C)CCCCCCCCCCCCCCCCCCCCCC

INSTITUTIONAL ASSESSMENT
COSING: ANNEX III

Similarity Index: 0,81

Final Class: only commercially available and with restrictions

Matching Function(s): HAIR CONDITIONING

Function: EMOLLIENT | EMULSION STABILISING | HAIR CONDITIONING | SKIN CONDITIONING

Molecule Name: DIMETHYL LAURAMINE ISOSTEARATE

CAS: 70729-87-2

SMILES: CCCCCCCCCCCCN(C)C.CC(C)CCCCCCCCCCCCCCCC(=O)O

VEGA SMILES:

INSTITUTIONAL ASSESSMENT
COSING: ANNEX III

Similarity Index: 0,8

Final Class: only commercially available and with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | PRESERVATIVE | ANTIMICROBIAL | DEODORANT | HAIR CONDITIONING | SURFACTANT

Molecule Name: LAURALKONIUM CHLORIDE | BENZALKONIUM CHLORIDE | COCOALKONIUM CHLORIDE

CAS: 139-07-1 | 8001-54-5

SMILES: [Cl-].CCCCCCCCCCCC[N+](C)(C)Cc1ccccc1

VEGA SMILES: c1ccc(cc1)C[N+](C)(C)CCCCCCCCCCCC

INSTITUTIONAL ASSESSMENT
COSING: ANNEX V

Similarity Index: 0,77

Final Class: only commercially available and with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | HAIR CONDITIONING

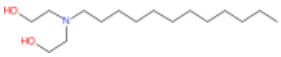
Molecule Name: DIBEHENYL METHYLAMINE

CAS: 61372-91-6

SMILES: CCCCCCCCCCCCCCCCCCCCCCN(C)CCCCCCCCCCCCCCCCCCCCCC

VEGA SMILES:
N(C)(CCCCCCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCCCC

INSTITUTIONAL ASSESSMENT
COSING: ANNEX III



Similarity Index: 0,75

Final Class: only commercially available and with restrictions

Matching Function(s): HAIR CONDITIONING

Function: HAIR CONDITIONING

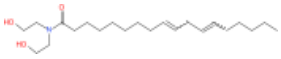
Molecule Name: N-LAURYL DIETHANOLAMINE

CAS: 1541-67-9

SMILES: CCCCCCCCCCCCN(CCO)CCO

VEGA SMILES:OCCN(CCO)CCCCCCCCCCCC

INSTITUTIONAL ASSESSMENT
COSING: ANNEX III



Similarity Index: 0,71

Final Class: only commercially available and with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | FOAM BOOSTING | HAIR CONDITIONING | VISCOSITY CONTROLLING

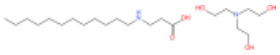
Molecule Name: LINOLEAMIDE DEA

CAS: 56863-02-6

SMILES: CCCCCC=CCC=CCCCCCCCC(=O)N(CCO)CCO

VEGA SMILES: O=C(N(CCO)CCO)CCCCCCCC=CCC=CCCCCC

INSTITUTIONAL ASSESSMENT
COSING: ANNEX III



Similarity Index: 0,7

Final Class: only commercially available and with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | CLEANSING | FOAM BOOSTING | HAIR CONDITIONING | SURFACTANT

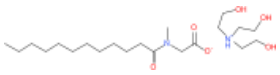
Molecule Name: TEA-LAURAMINOPROPIONATE

CAS: 14171-00-7

SMILES: CCCCCCCCCCCCNCCC(=O)O.OCCN(CCO)CCO

VEGA SMILES:

INSTITUTIONAL ASSESSMENT
COSING: ANNEX III



Similarity Index: 0,68

Final Class: only commercially available and with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | CLEANSING | FOAMING | HAIR CONDITIONING | SURFACTANT

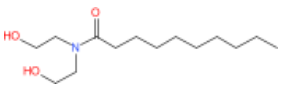
Molecule Name: TEA-LAUROYL SARCOSINATE

CAS: 16693-53-1

SMILES: CCCCCCCCCCCC(=O)N(C)CC(=O)[O-].OCC[NH+](CCO)CCO

VEGA SMILES:

INSTITUTIONAL ASSESSMENT
COSING: ANNEX III



Similarity Index: 0,68

Final Class: only commercially available and with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | FOAM BOOSTING | HAIR CONDITIONING | SURFACTANT | VISCOSITY CONTROLLING

Molecule Name: CAPRAMIDE DEA

CAS: 136-26-5

SMILES: CCCCCCCCCC(=O)N(CCO)CCO

VEGA SMILES: O=C(N(CCO)CCO)CCCCCCCCC

INSTITUTIONAL ASSESSMENT
COSING: ANNEX III

Similarity Index: 0,68

Final Class: only commercially available and with restrictions

Matching Function(s): HAIR CONDITIONING

Function: ANTISTATIC | CLEANSING | FOAMING | HAIR CONDITIONING | SURFACTANT

Molecule Name: TEA-OLEOYL SARCOSINATE

CAS: 17736-08-2

SMILES: CCCCCCCCC=CCCCCCCCC(=O)N(C)CC(=O)O.OCCN(CCO)CCO

VEGA SMILES:

INSTITUTIONAL ASSESSMENT
COSING: ANNEX III

No BANNED OR NOT RECOMMENDED compounds found in DB