

Complementary Green Analytical Procedure Index (ComplexGAPI) and Software

Supporting Information: Software Documentation

Justyna Płotka-Wasyłka^{1*} and Wojciech Wojnowski¹

¹Department of Analytical Chemistry, Faculty of Chemistry, Gdańsk University of
Technology, 11/12 G. Narutowicza Street, 80-233 Gdańsk, Poland

*juswasyl@pg.edu.pl

Contents

1 Introduction	1
2 Disclaimer	2
3 Installation	2
4 User Interface	2
5 GAPI and ComplexGAPI criteria	3
5.1 Parameter I	4
5.2 Parameter III	4
6 Bibliography	4

1 Introduction

The ComplexGAPI software is intended to aid the user in determining the Green Analytical Procedure Index (GAPI) and its modification, the Complementary Green Analytical Procedure Index (ComplexGAPI). It is intended as a simple, standalone, GUI-based tool for generating pictograms which highlight the processes in an analytical procedure which could be improved from the point of view of Green Analytical Chemistry. The pictograms can also be used to juxtapose the developed method with other methods in terms of environmental impact.

The calculator was developed in Python 3.8 using the Tkinter module [1].

2 Disclaimer

This software is provided “as is,” and any express or implied warranties, including but not limited to the implied warranties of merchant-ability and fitness for a particular purpose, are disclaimed. In no event shall the authors be liable for any direct, indirect, incidental, special, exemplary, or consequential damages (including, but not limited to, procurement of substitute goods or services; loss of use, data, or profits; or business interruption) however caused and in any way theory of liability, whether in contract, strict liability, or tort (including negligence or otherwise) arising in any way out of the use of this software, even if advised of the possibility of such damage.

This software is made available under the MIT license.

3 Installation

The most recent code can be obtained from the open repository, which is maintained at git.pg.edu.pl/p174235/complexgapi.

A compiled, stand-alone version is currently available for Windows and can be downloaded from mostwiedzy.pl/complexgapi. The downloaded file is a self-extracting archive. The user will be asked to indicate the destination folder (see Figure S1). After extraction, the application can be launched by running the *ComplexGAPI.exe* executable located in the extracted archive.

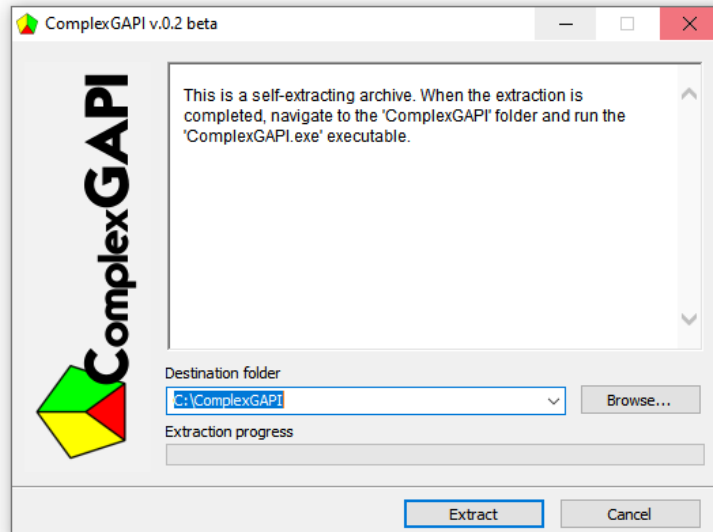


Figure S1: The SFX dialog.

4 User Interface

The user interface is shown in Fig. S2. The highlighted elements are:

1. File menu containing a “Save image” option which invokes the system file manager and enables exporting either the GAPI pictogram or the ComplexGAPI pictogram as either a raster (.png) or vector (.svg) file, and an info page;
2. The sample preparation and analysis pane – if only these dialogs are selected, the result will be the original GAPI pictogram;
3. The Pre-analysis processes pane – the added functionality of ComplexGAPI;
4. Hyperlink to a popup window containing a table listing the Green Economy rules;
5. Pictogram preview area updated in real-time.

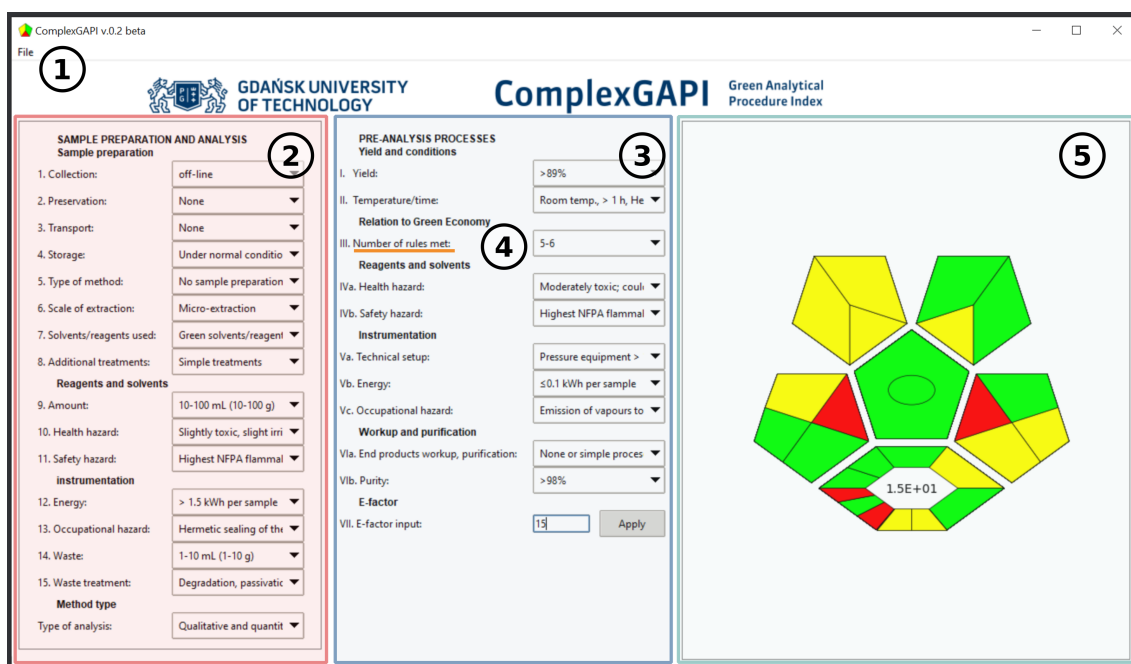


Figure S2: Main GUI elements; the coloured areas are superimposed as highlights of the referenced elements, and are not a part of the actual GUI.

5 GAPI and ComplexGAPI criteria

The parameters associated with the evaluated analytical procedure are selected from the drop-down menus in the main window (Fig. S2 elements 2 and 3). The corresponding fields in the pictograph preview are assigned the corresponding colour (green, yellow, or red) based on the criteria outlined in the ComplexGAPI tool. Parameter III (the number of the rules of Green Economy which are met) is a compound score based on the rules outlined in Table S1, which can also be displayed within the software by clicking on the parameter itself. Additionally, the value of parameter VII (the E-factor) is provided by the user and displayed in the central field of the graph in scientific notation rounded to the first decimal point.

5.1 Parameter I

In Parameter I, the User is asked to select the appropriate option from the drop-down menu based on the yield/selectivity of the assessed procedure. These can be calculated based on the following equations:

$$\%Yield = \frac{\text{product moles}}{\text{limiting reactant moles}} \times 100 \quad (\text{Equation 1S})$$

$$\%Conversion = \frac{\text{limiting reactant final mass}}{\text{limiting reactant initial mass}} \times 100 \quad (\text{Equation 2S})$$

$$\%Selectivity = \frac{\%Yield}{\%Conversion} \times 100 \quad (\text{Equation 3S})$$

5.2 Parameter III

Parameter III (the number of the rules of Green Economy which are met) is a compound score based on the rules outlined in Table S1, which can also be displayed within the software by clicking on the parameter itself.

Table S1: Rules of Green Economy and the corresponding points for Parameter III.

Requirement	Green chemistry component	Points	Result in the economy of synthesis/reaction/process
Design	Application of experimental design to reduce or eliminate the use or generation of hazardous substances	1	It aids in finding methods and techniques to speed up chemical reactions using small amounts of reagents to produce equivalent results at the same price point.
	Assessment of the chemical product's life cycle, including its design, manufacture, use, and ultimately disposal	1	It might also lead to reduction of the number of synthetic steps and result in increased production and plant capacity while reducing energy and water consumption
Use	Use of raw materials, elimination of waste and avoiding the use of toxic and/or hazardous reagents and solvents	1	It aids in finding methods and techniques to speed up chemical reactions using small amounts of reagents to produce equivalent results at the same price point.
	Prevention of pollution by waste minimization and avoidance of toxic and hazardous substances	1	Using fewer chemicals for products manufacture results in reduced waste, which in turn reduces the cost of disposing and treatment of chemical waste
Effort	Effort to minimize expenditure of energy and chemicals	1	Using fewer chemicals for products manufacture results in reduced waste, which in turn reduces the cost of disposing and treatment of chemical waste
	Effort to use harmless reactants, alternative solvents, and new pathways of synthesis	1	

6 Bibliography

- [1] Python Software Foundation. Tkinter - Python interface to Tcl/Tk - Python 3.7.7 documentation. <https://docs.python.org/3.7/library/tkinter.html>. Accessed: 2020-04-02.