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ChlorTox Base – a useful source of information on popular reagents in terms of chemical hazards and greenness assessment

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ABSTRACT

ChlorTox Base is a database on the chemical hazards of popular reagents used in the chemical laboratory, derived from available safety data sheets published by various manufacturers. 1,388 sheets and 674 different chemicals were reviewed. Weighted hazards number (WHN) was used as the main parameter reflecting the "greenness" of particular substances, understood as a spectrum and severity of various forms of adverse health, safety, and environmental impacts. The presented WHN values can be directly used in the greenness assessment and evaluation, for instance in the ChlorTox Scale – a simple tool for estimating chemical risk of laboratory method in accordance with the postulates of the Unified Greenness Theory.

1. Introduction

1.1. Preface

Exposure to the hazards associated with the use of chemicals, including their adverse impact on user health and the environment, is an integral part of chemistry as a field of science and industry. We can ask ourself, are we aware of these hazards in everyday life? Are we able to assess when the potential risk is higher and when lower, which reagent is potentially more dangerous and which is less? On what basis can we objectively state this? How to use knowledge about chemical hazards in assessing the greenness of chemical procedures and products? This article and the presented ChlorTox Base may be a partial answer to these questions. The data presented may be useful to anyone who has any contact with the chemical reagents to identify the risk, as well as anyone interested in green chemistry and performing greenness evaluation.

1.2. Selected postulates of the Unified Greenness Theory

The basic theoretical assumptions of green chemistry including both synthesis and analysis (green analytical chemistry), have recently been formulated as the Unified Greenness Theory (UG-theory) [1]. One of its postulates is the mathematical definition of greenness, according to which:

"Greenness can be represented mathematically as a set of elemental effects of different nature."

$$G = \{E_1,\ E_2,\ \ldots,\ E_n\} \tag{1}$$

Where G is the greenness indicator of the object (product, process, method), E is the elemental effect of a destructive influence on the environment and/or human, caused directly or indirectly by this object, and n is the number of all elemental effects that can be identified at a given moment. G is inversely proportional to greenness, and proportional to harm (destructive impact).

Five elemental effects were identified:

$$G = \{CF,\ CC,\ EE,\ PI,\ IE\} \tag{2}$$

Where *CF* is Carbon Footprint (the emission of greenhouse gases that cause climate change), *CC* is Chemical Contamination (the entire chemical impact of substances used on the environment and process operator), *EE* is Earth Exploitation (irreversible devastation of all Earth's resources), *PI* is Physical Impact (injuries and harms sustained by exposure to physical factors), and *IE* is Infections & Epidemics (infections with pathogens that are dangerous to health and life, and resulting epidemics). UG-theory goes on to say that:

Abbreviations: ChlorTox Scale, Chloroform-oriented toxicity estimation scale; DES, deep eutectic solvent; UG-theory, Unified greenness theory.

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"Elemental effects, i.e., *the so-called elements of greenness, are functions of three basic variables: the severity of hazard, the amount of the factor posing a hazard, and the effectiveness of counteracting the hazard."*

$$E = f(h,\ q,\ p) \tag{3}$$

Where h means the severity of hazard which depends on the characteristics of a given factor, q means the quantity of this factor, and p means the effectiveness of counteracting the hazards (prevention).

Regarding greenness assessment, the UG-theory differentiates methods from method application process, and states that:

"Methods can be assessed and evaluated in terms of only two of the three essential variables: the severity of hazard and the quantity of factor posing that hazard. The degree of prevention cannot be assessed objectively as it depends on the individual circumstances of the method application process."

This statement comes from the fact that method protocol indicates what hazardous factors and in what quantities should be used, but does not specify the effectiveness of protection against individual hazards. For example, protection against contact and release of chemicals and waste is governed by separate procedures.

Thus, the correlation between the hazard (h) and its quantity (q) can be defined as "the risk of a destructive effect caused by the use of a particular method (procedure), under unspecified circumstances":

$$R = f(h, q) \tag{4}$$

Where R is the degree of this risk.

The unit risk associated with a single factor is in approximation the product of these two variables:

$$R' = h \cdot q \tag{5}$$

Where R' is the estimated degree of unit risk caused by a single factor.

1.3. ChlorTox Scale

Chloroform-oriented Toxicity Estimation Scale (ChlorTox Scale) is a greenness indicator relating to the *CC* element, proposed recently in the literature [2], fully compatible with the UG-theory [1]. This is a new approach aimed at estimating the chemical risk of any laboratory method/procedure in a comprehensive but still very simple way. The basis of this approach is to refer hazards related to the substance-of-interest to the hazards identified for the standard substance – chloroform (it indicates the h variable), and to consider the precisely known mass of the substance used in the method (q variable). The results are expressed in equivalent mass of chloroform, indicating the degree of estimated chemical risk, see Fig. 1.

It requires the use of the following simple equation:

$$\text{ChlorTox} = \frac{CH_{sub}}{CH_{CHCl3}} \cdot m_{sub} \tag{6}$$

Where the ChlorTox value, expressed in the mass of chloroform [g], reflects a degree of chemical risk associated with the substance-of-interest, taking into account its properties (hazards) and the amount used. CH_{sub}/CH_{CHCl3} represents a relative hazard of using the assessed substance in relation to chloroform, assuming the same mass-to-volume concentration of both chemicals, and m_{sub} is a mass of the substance-of-interest needed to apply the method (other details are presented in the original paper [2]).

The ChlorTox values characterizing different substances can be added together to express the total chemical risk predicted for the whole method (Total ChlorTox). The ChlorTox value has a purely theoretical meaning, it is not directly reflected in reality, but it indicates the general scale of potential risk. For example, a method with a Total ChlorTox value of 1 g poses a risk which is analogous to a method using 1 g of pure chloroform per one analysis as the only dangerous chemical reagent.

To facilitate rapid evaluation of the method using the ChlorTox Scale, a simple model for quantifying general chemical hazard was developed, called the Weighted Hazards Number (WHN) [2]. It consists in searching for relevant information on the hazards posed by given chemical reagents in publicly available safety data sheets, presented in the commonly used Globally Harmonized System of Classification and Labeling of Chemicals (GHS) format. This system covers hazards associated with storage and transport, direct health hazards (poisoning, chemical burns, irritation, carcinogenicity) and environmental hazards (impact on model species of microorganisms, plants, and animals). In addition, there are categories denoting the degree of hazard, the number of which, depending on the type of hazard, ranges from 1 to 4. Category 1 means the highest degree of hazard (the greatest potential danger), while 4 the least. This information is always presented in the Section 2 (Hazards identification).

For example, for chloroform offered by Sigma-Aldrich one can find the following information [3]: Acute toxicity, Oral (Category 4), H302.

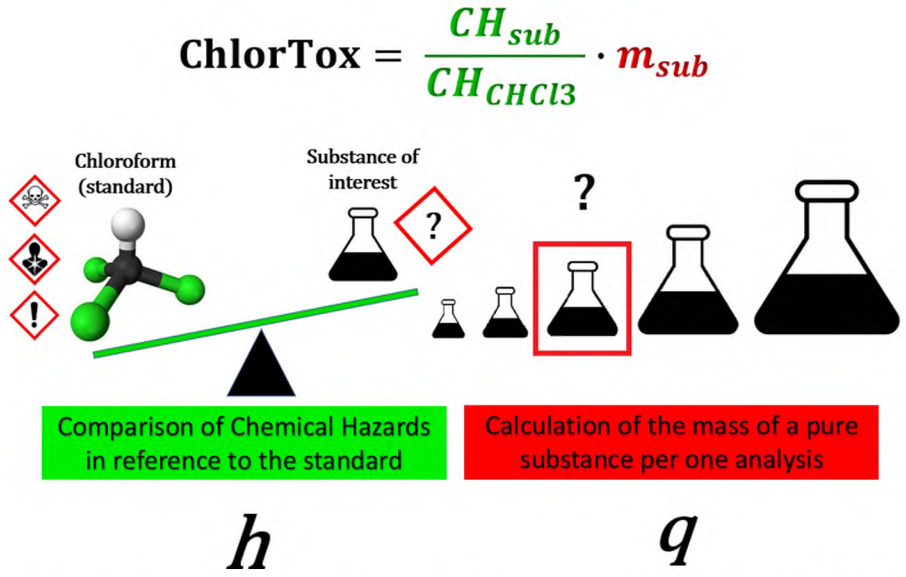

Fig. 1. The idea of assessing the chemical risk of a laboratory method using the ChlorTox Scale, based on two variables: h (Chemical Hazard) and q (mass).

Acute toxicity, Inhalation (Category 3), H331. Skin irritation (Category 2), H315. Eye irritation (Category 2A), H319. Carcinogenicity (Category 2), H351. Reproductive toxicity (Category 2), H361. Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336. Specific target organ toxicity - repeated exposure, Oral (Category 1), Liver, Kidney, H372. Short-term (acute) aquatic hazard (Category 3), H402. Thus, nine hazards in total have been identified, of which one is category 1, four are category 2, three are category 3 and one is category 4.

In the WHN approach, the overall hazard of the substance-of-interest (CH_{sub}) and chloroform (CH_{CHCl3}) is expressed by *WHN* value. *WHN* is determined as the sum of the hazards identified in the Section 2 of the safety data sheets (GHS format), with weights reflecting the degree of potential danger (hazard category): 1 for category 1, 0.75 for category 2, 0.5 for category 3 and 0.25 for category 4:

$$WHN\ (CH_{sub}) = 1 \cdot N_{cat1} + 0.75 \cdot N_{cat2} + 0.5 \cdot N_{cat3} + 0.25 \cdot N_{cat4} \quad (7)$$

where N_{cat} is the number of hazards of a given category.

For chloroform, according to the data provided by Sigma-Aldrich [3]:

$$WHN\ (CH_{CHCl3}) = 1{\cdot}1 + 0.75{\cdot}4 + 0.5{\cdot}3 + 0.25{\cdot}1 = 5.75 \quad (8)$$

To ensure reliable method assessment with the WHN model, the recommendation was proposed to select one preferred safety data supplier for the whole assessment process [2].

1.4. Why ChlorTox Base?

The purpose of this article is to collect data on the chemical hazards of the most popular reagents used in analytical laboratories in the form of an open database called ChlorTox Base, to improve the consistency and objectivity of the results obtained with the ChlorTox Scale and other greenness and whiteness metric tools [4–12]. Notably, the hazard data provided by different manufacturers can vary quite significantly, and selecting one preferred data supplier for all reagents used in a method is not an optimal solution. This issue can be difficult and debatable. The aim of the ChlorTox Base is to clearly indicate the specific CH_{sub} and CH_{CHCl3} values that should be used in the ChlorTox Scale based on the WHN model Eqs. (6), ((7) and (8)). Besides omitting the need to choose the preferred data supplier which can be a quite subjective decision, it eliminates the need to do one's own research on hazard data and thus simplifies assessment procedure. ChlorTox Base presents also a range of interesting details to analyze and compare reagents from different angles. An Excel spreadsheet containing the first version of ChlorTox Base (1.0) is included as a supplement to this publication. The method of data selection and the most important conclusions from the analysis of the presented data are described below.

2. Data selection key

The data used to create ChlorTox Base came from the safety data sheets (GHS format), obtained through the search engine available on chemicalsafety.com [13]. All sheets found by this webservice were carefully verified. Only data relating to the pure forms of given substances were presented in the database (without mixtures and dilutions). The most up-to-date versions provided by a given data supplier were used. Data published earlier than in 2020 was not taken into account, so that the picture of the hazards posed by individual substances was as up-to-date and correct as possible. In total, 1388 safety data sheets were used to create ChlorTox Base, referring to a total of 674 different chemical reagents. This collection includes reagents currently stored in the didactic and research laboratories of the Department of Analytical Chemistry, Faculty of Chemistry, Jagiellonian University in Krakow. It has been additionally enriched with selected substances belonging to ionic liquids and deep eutectic solvents (DES) components, which are currently very popular [14–16].

3. ChlorTox Base description

3.1. "Whole database" sheet

The first sheet of ChlorTox Base ("Whole Database") contains all the relevant data, such as: chemical name of the individual reagent, CAS number, category (organic or inorganic), subcategory (solid, liquid, ionic liquid, DES component), molar mass, name of the safety data supplier, the date of updating the data contained in the sheet, a direct link to the sheet (pdf file), as well as a number of data corresponding to hazards. These are: the number of hazards assigned to a given category (Eq. (7)), all *WHN* values obtained for a given reagent, average *WHN*, standard deviation and relative standard deviation of *WHN* for a given reagent (showing the discrepancy of data obtained from different sources), number of pictograms, average number of pictograms for a given reagent, word code (none, warning, or danger), number of precautionary statements, and average number of precautionary statements for a given substance.

3.2. "ChlorTox Scale application" sheet

The second sheet ("ChlorTox Scale Application") presents key data for the application of the ChlorTox Scale. It was assumed that the most consistent and reliable results will be obtained by using the arithmetic mean of all *WHN* values for a given reagent collected in the database, coming from various sources (data suppliers). In consequence, the average *WHN* values obtained for chloroform (standard) and other substances should be used in Eq. (6) as CH_{CHCl3} and CH_{sub}, respectively. To keep clarity, the second sheet only presents name of chemical, CAS number, and the average *WHN* value to be used in Eq. (6).

It is worth noting here that the average *WHN* value for chloroform equals 5.83 and is slightly different from the value obtained previously for the data provided by Sigma-Aldrich (5.83 v 5.75). According to the ChlorTox Base idea, the averaged and standardized *WHN* value can be considered more reliable than that coming from only one subjectively selected source.

It is obvious that it is impossible to include all possible reagents in the database. In the absence of data on a given chemical substance in ChlorTox Base, we recommend finding the missing information on one's own using the chemicalsafety.com portal or another search engine [13]. For consistency, it is recommended to take an average *WHN* based on data published no earlier than 2020. When multiple sheets are available from the same data supplier, we recommend using the most recent one. In the absence of safety data sheets, for example, for new and less popular reagents, we recommend estimating the hazard in a different way, for example by referring to another substance that is closest in terms of properties (more on this problem in [2]).

3.3. Other sheets

The other sheets contain the results of the data analysis performed based on the "Whole Database" sheet, such as graphs showing potential correlations between selected parameters. Their description is presented in the next section.

4. Analysis of data collected in the ChlorTox Base

4.1. Most hazardous chemicals

The general picture of the results obtained for all analyzed safety data sheets is presented in Fig. 2. For the purposes of this analysis, data obtained for the same reagent on the basis of different safety data sheets are treated individually (without averaging the *WHN* values).

Undoubtedly, the most interesting question may be which reagent

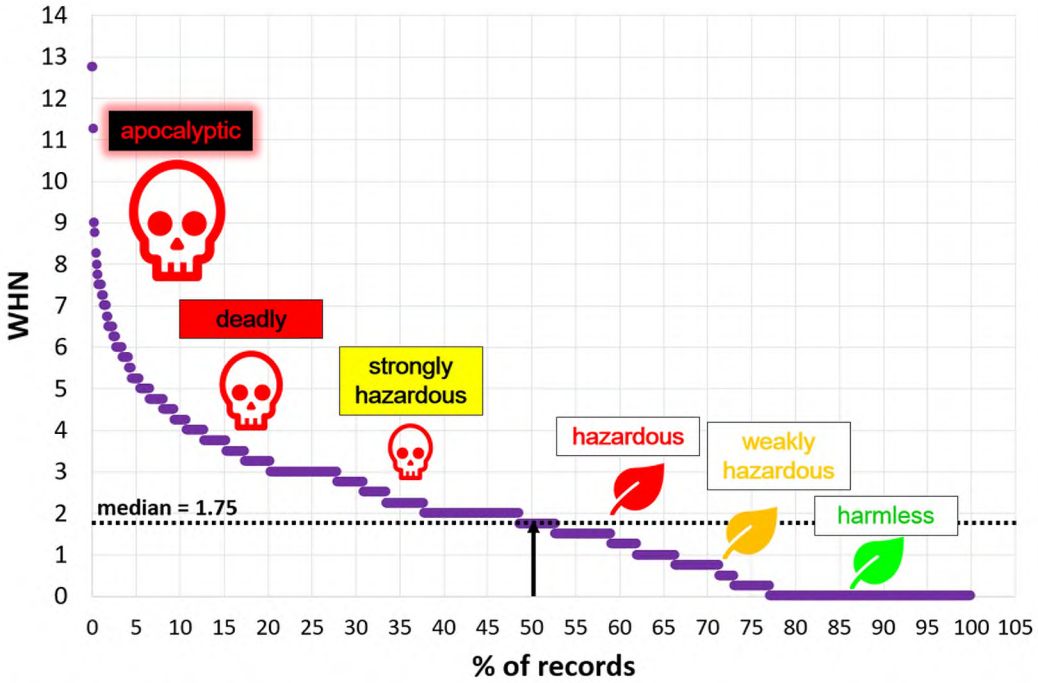

Fig. 2. Percentage of records with a given WHN value in the entire ChlorTox Base (WHN values obtained for one reagent based on safety data from different sources are treated as separate records). The higher the WHN value, the greater the total chemical hazard posed by the substance. The proposed classification and labels are only auxiliary and are a subjective expression of authors emerged upon analyzing the collected data and realizing how dangerous are some chemicals.

turned out to be the most dangerous in the overall sense, which is reflected in the highest *WHN* value. It turns out that this reagent is a popular inorganic chromium salt - potassium dichromate, which obtained *WHN* values of 12.75 (according to data provided by Sigma-Aldrich), 12.75 (Thermo Fisher), and 11.25 (Panreac Quimica). It is worth emphasizing that no other reagent has achieved a *WHN* value above 10, which shows how many different health and environmental hazards are posed by potassium dichromate. Its spectrum of adverse effects is truly huge, which we may not be fully aware of when we encounter this substance in the laboratory (details on all hazards are available in the safety data sheets, links to which are included in the attached Excel file). Further places in the infamous ranking are taken by: cobalt(II) nitrate hexahydrate (WHN=9) ex aequo with 1,1,1-trichloroethane, aniline (WHN from 8 to 8.75), and tin(II) chloride (WHN=7.75) ex aequo with phenol, hexane, trichloroethylene, benzene and epichlorohydrin (see Excel file for more information).

In addition, it is worth noting that the average *WHN* value for all records in the database is 1.94, whereas the median 1.75, moreover, 23% of the records have a zero *WHN* value, i.e. they concern substances for which no hazard was found in the safety data sheets (it is nicely seen in Fig. 2).

4.2. Division into selected groups – comparison

In this analysis, the reagents were grouped by selected keywords to compare the average *WHN* values obtained for the particular groups, as shown in Table 1.

First, we note that organic reagents make up the vast majority of all chemicals gathered in the ChlorTox Base, and the average *WHN* value for them is lower than for inorganic ones (1.82 vs 2.50), which is in their favor. This may simply be due to the fact that we ourselves consist mostly of organic compounds, a large part of which is relatively neutral both for us and the environment. We also see that liquids have a similar share in the base as solids, and the average *WHN* values do not differ significantly for them (2.03 vs 1.83). Interestingly, the DES components have a similar average *WHN* value as all substances considered together (1.92 vs 1.94), and the ionic liquids have a relatively slightly lower value (1.30). However, this result should be interpreted with caution, because compared to frequently used organic solvents, these values are still relatively low.

Table 1
The number of records and the average WHN value for a selected group of chemicals found in the ChlorTox Base using a given keyword.

Keyword		Records number	Average WHN
All chemicals		1388	1.94
Category	"inorganic"	171	2.50
Category	"organic"	1217	1.86
Sub-category	"liquid"	742	2.03
Sub-category	"solid"	645	1.83
Sub-category	"DES component"	108	1.92
Sub-category	"ionic liquid"	279	1.30
SDS supplier	"Sigma-Aldrich"	495	2.00
SDS supplier	"Combi-Blocks"	398	1.33
SDS supplier	"Thermo Fisher"	348	2.43

SDS supplier means safety data sheet supplier.

It is also worth noting that the main suppliers of safety data, i.e. Sigma-Aldrich, Combi-Blocks and Thermo Fisher, are responsible for 1242 out of 1388 records in the entire database. The average *WHN* values obtained for data from individual suppliers differ quite significantly. On the one hand, this may indicate a lack of consistency in the assessment of hazards between individual entities, which would be quite a worrying phenomenon, but on the other hand, it should be borne in mind that the compared *WHN* values do not refer to the same set of substances, which certainly explains some of the observed discrepancies. Nevertheless, after a thorough analysis of the data collected in the ChlorTox Base ("Whole database" sheet), it can be clearly stated that a certain discrepancy exists, and in some cases, it is alarmingly large. For example, for chloroform, which serves as a reference substance in the ChlorTox Scale, *WHN* values range from 4.75 (Panreac Quimica) to 7.00 (Thermo Fisher). This is hard evidence that in order to increase the consistency and objectivity of the greenness assessment with the ChlorTox Scale, it is better to always use the average *WHN* values

provided in the ChlorTox Base rather than relying on one selected data supplier.

4.3. Potential correlation between selected parameters

Recall that in the ChlorTox Scale approach, the *WHN* value is calculated taking into account all the hazards listed in Section 2 of the safety data sheet, taking into account the severity of the hazard given by the category (Eq. (7)). The purpose of this section is to verify whether and how the *WHN* value correlates with other parameters reported in the safety data sheets, which can also be considered as indicators of the general hazard (toxicity) of chemicals. These include: the total number of hazards (without taking into account the category indicating their severity) – see Fig. 3A, the total number of hazard pictograms – Fig. 3B, and the total number of precautionary statements that match the characteristics of the considered substance – Fig. 3C.

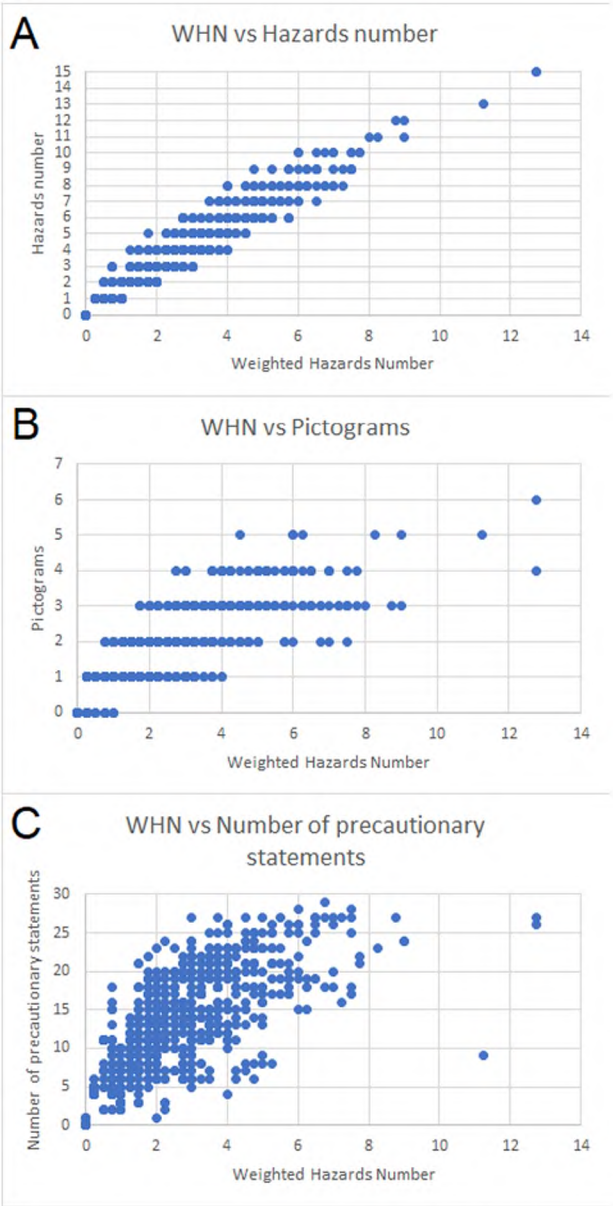

Fig. 3. Selected parameters related to the chemical hazard given in the safety data sheets: (A) number of hazards (not including categories), (B) number of pictograms, and (C) number of precautionary statements; as a function of WHN (weighted hazards number including hazard categories).

As it results from Fig. 3A, taking into account the hazard category is of great importance, as evidenced by the relatively large discrepancies in the *WHN* values obtained for the same values of the unweighted (ordinary) number of hazards. Although the use of a simpler formula and the rejection of weights could further simplify the use of the ChlorTox Scale, the consequence could be the loss of some important information and a decrease in the objectivity of the assessment. Similar conclusions can be drawn by analyzing the relationship between the number of pictograms and *WHN* – Fig. 3B. Unsurprisingly, the discrepancies are even greater, which proves that relying "only" on pictograms is a very far-reaching simplification and does not reflect the real characteristics of chemical hazards. Third, a certain correlation can be found between the total number of recommended precautionary statements and *WHN* – Fig. 3C. This indicator may seem quite precise and strictly related to the characteristics of a given substance and its impact on humans and the environment. Indeed, in some cases the number of precautionary statements reaches almost 30. Notably, in the case of potassium dichromate, this number exceeds 25, which proves the highly dangerous nature of this substance. The conclusion is that this indicator can be a useful parameter to describe the risk profile of a given reagent for more comprehensive greenness assessment with the ChlorTox Scale, using a more complex chemical hazard expression model than WHN [2]. This model could also take into account *WHN* values, number of pictograms and word code (none, warning, or danger) given by manufacturers in safety data sheets. All these parameters could to be considered as complementary to each other. In the basic approach, however, adding additional parameters to Eqs. (6) or (7) does not seem advisable due to the complication of the whole procedure and potential loss of user-friendliness.

4.4. WHN versus acute toxicity (LD_{50})

It should be emphasized that the *WHN* value is an expression of the spectrum of adverse impacts of various nature, also taking into account the severity of particular hazards expressed by categories (from 1 to 4). This parameter cannot be equated with a measure of one specific hazard, for example acute toxicity after ingestion, expressed by the LD_{50} parameter. As can be seen from Table 2, there is no direct correlation between *WHN* and LD_{50}, confirming that these parameters cannot be used interchangeably because they describe different issues. With regard to the assessment of greenness, *WHN* seems to be a better indicator than LD_{50} because it describes chemical substance from a general perspective and depends on many different ways of destructive impact on health and environment. At the same time, it should be stated that *WHN* is not an ideal indicator, it is a kind of compromise between the objectivity of the assessment and the simplicity of its determination and use.

5. Conclusions

Almost 700 chemical reagents used in analytical chemistry laboratories have been characterized in terms of chemical hazards, based on the most updated versions of safety data sheets from various manufacturers. The most important parameter is the average *WHN* value obtained for a given reagent, which is a measure of how severe the spectrum of adverse effects on humans and the environment is. We recommend using these values in the ChlorTox Scale method, to facilitate this, they have been clearly shown in the "ChlorTox Application" sheet, in the attached Excel file containing ChlorTox Base 1.0. The current version of database is not complete, it is impossible to put all the reagents in it. However, its systematic development and enrichment with new substances are planned in the future. The use of ChlorTox Base may allow for greater consistency and objectivity in the assessment of greenness of methods with different profiles, not excluding chemical synthesis methods. One should be aware of the multitude of hazards and danger resulting from the use of substances with the highest *WHN* values. Dissemination of knowledge on this subject in necessary,

Table 2
Comparison of WHN and acute toxicity expressed by LD_{50} values (oral administration, rat or mouse as a model), for the most hazardous substances according to the ChlorTox Base, and some arbitrarily selected additional popular reagents used in the laboratory, according to the data provided by Sigma-Aldrich.

Name of chemical	Weighted hazards number	LD_{50} (g/100 kg)
Potassium dichromate	12.75	9.1
Cobalt(II) nitrate hexahydrate	9	97.8
Aniline	8.25	25.0
Tin(II) chloride	7.75	191.0
Benzene	7.5	200.0
Cadmium chloride	7.25	10.7
Potassium chromate	7	no data
Phenol	6.5	10.0
Ethylenediamine	6.5	86.6
Warfarin	6.5	0.2
Epichlorohydrin	6.5	17.5
1-Naphthol	6.25	150.0
Carbon tetrachloride	6.25	235.0
Hexane	6	1600.0
Xylenes	6	352.3
Propylamine	6	37.0
Tetrabutylphosphonium bromide	6	42.0
Benzyltriphenylphosphonium chloride	6	4.3
Furfural	6	10.8
Chloroform (standard)	5.75	90.8
Cypermethrin	5.75	50.0
Toluene	5.75	558.0
Silver nitrate	5.75	380.4
(−)-Nicotine	5.5	5.0
Cyclohexane	5	500.0
Methyl formate	4.75	10.0
Zinc chloride	4.25	110.0
Copper(II) chloride	4	58.4
Carbamazepine	3.25	195.7
Formic acid	3.25	73.0
Phosphoric acid	3.25	125.0
Acetic acid	2.5	331.0
Acetonitrile	2.25	61.7
Acetone	2	580.0
Ethanol	1.5	1047.0
Calcium chloride	0.75	no data
Ammonium formate	0.75	225.0
Caffeine	0.75	36.8
Urea	0	847.1
Glycine	0	793.0

Note that toxicity is inversely proportional to LD_{50}. The source data are presented in the attached Excel file.

especially among inexperienced students who have frequent contact with these substances in the course of their studies. If you have any questions or concerns regarding ChlorTox Base and ChlorTox Scale, please contact us by e-mail, we are ready to help.

CRediT authorship contribution statement

Paweł Mateusz Nowak: Conceptualization, Methodology, Formal analysis, Supervision, Writing – original draft, Writing – review & editing, Funding acquisition. **Alicja Bis:** Data curation, Methodology. **Aleksandra Zima:** Data curation, Methodology.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

All data supporting the manuscript content are available in the attached Excel file.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.greeac.2023.100065.

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