

## DOZN™ – A Quantitative Green Chemistry Evaluator

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**ABSTRACT**

MilliporeSigma created a unique web-based greener alternative scoring matrix, also known as DOZN™ a quantitative green chemistry evaluator based on the 12 principles of green chemistry. The 12 principles of green chemistry provide a framework for learning about green chemistry and designing or improving materials, products, processes and systems. DOZN™ scores products based on metrics for each principle and aggregates the principle scores to derive a final aggregate score. The system calculates scores based on manufacturing inputs, Globally Harmonized System (GHS) and Safety Data Sheet (SDS) information which provide a green score for each substance. DOZN™ is flexible enough to encompass the diverse portfolio of products ranging from chemistry to biology based products. The DOZN™ system has also been verified and validated by a third party to ensure best practices are applied. This new Greener Chemistry initiative offer customers 'an increased breadth of Greener Alternative products with confirmatory documentations to validate greener characteristics.

**Keywords**

Green Chemistry Matrix, Greener Alternative Products, Human Health, Twelve Principles of Green Chemistry.

**Introduction**

Green chemistry is the concept of developing chemical products and processes that reduce the use and generation of hazardous materials, minimize waste, and reduce demand on diminishing resources. Paul Anastas and John Warner developed the framework that has served as the foundation for a global framework for green chemistry [1]. That framework proposes 12 complementary principles around resource efficiency and risk (human health and environmental) minimization, targeting a life-cycle perspective (e.g., raw materials extraction, chemical production, and end-of-life bioaccumulation and biodegradation). These 12 principles were also adopted by American Chemical Society (ACS) Green Chemistry Institute (GCI) [2]. The 12 principles are as follows:

- Prevent Waste
- Atom Economy
- Less Hazardous Synthesis
- Design Benign Chemicals
- Benign Solvents & Auxiliaries

- Design for Energy Efficiency
- Use of Renewable Feed-stocks
- Reduce Derivatives
- Catalysis (vs. Stoichiometric)
- Design for Degradation
- Real-Time Analysis for Pollution Prevention
- Inherently Benign Chemistry for Accident Prevention.

While various approaches to quantifying greener processes and products have been proposed, there is no unifying set of metrics in place. After a review of the current state of green chemistry methods, MilliporeSigma developed DOZN™, a quantitative green chemistry evaluator and leveraged generally accepted industry practices. In review of the literature, we found that while a number of methods have been proposed to evaluate greener chemistry, there are hindrances to their implementation. Primary limitations include requiring a high level of effort [3-5], data that are not readily available [4,5], and access to specialized or proprietary data sets [4-6]. Additional limitations include results that lack transparency and are difficult to communicate [6]. Furthermore, some methods focused on a subset of stewardship principles, rather than endeavoring to capture the full suite of the 12 principles [3,5].

One example of a method to evaluate green chemistry is the iSUSTAIN Green Chemistry Index developed by Beyond Benign, Sopheon, and Cytec Industries Inc. [6]. This method provides an approach to generate a sustainability-based score for chemical products and processes following the 12 principles. iSUSTAIN provides a gate-to-gate assessment, whereas the DOZN™ approach permits the company to set the assessment boundaries depending on flexibility of available information, such as expanding the boundaries to include product use or disposal. The iSUSTAIN assessment uses a proprietary database to provide safety, health, and environmental information for common raw materials, solvents, diluents, and other auxiliary materials. Data for new materials can be requested from iSUSTAIN. The specialized database is then used to populate formulas for each principle. Depending on the principle, scores are tabulated or normalized on a scale of 0 to 100 to put them on the same scale, making them additive. The ability to combine principles into a single score may mislead the user to consider the principles to be comparable and make comparing alternatives less transparent.

Another approach to evaluating green chemistry is the NSF/GCI/ANSI 355-2011 standard, developed by the NSF International (NSF), GCI, and American National Standards Institute (ANSI) [3]. Broadly, this standard provides guidance to report chemical characteristics (human health effects, toxicology, ecological impacts, and physical safety properties), chemical processes (resource efficiency, recycled or bio-based materials, waste, water, energy), and social responsibility. While the NSF/GCI/ANSI 355-2011 standard was designed to improve communication and comparability of chemicals, it does not provide a method for tabulating scores to determine which chemical characteristics are less harmful to the environment and puts the onus on the customer. It also does not strictly follow the 12 principles in that it excludes chemical use and end-of-life stages and the specific principles of reduce derivatives, use of catalysis, design for degradation, and real-time analysis for pollution prevention.

A recent development in green chemistry is the California Safer Consumer Products Regulations (SCP regulations) [7]. This regulation requires application of an alternative analysis that can be used to compare an existing product-chemical combination that contains a chemical of concern to a safer alternative. The Draft Alternative Analysis Guide [4] includes 16 relevant factors at various stages of the product's lifecycle. Many of these relevant factors namely the adverse public human health impacts, adverse environmental impacts, physical chemical hazards, adverse waste and end-of-life effects, materials and resource consumption impacts, and renewable resources consumption follow themes similar to the 12 principles. The Draft Alternative Analysis Guide provides high-level guidelines on how to identify relevant factors, screen alternatives, assess lifecycle impacts, and compare alternative chemicals, but it does not provide a method for tabulating scores to determine which alternative chemical is less harmful to the environment. The onus is put on the responsible entity to make decisions to either implement an alternative or retain the original priority product alternative. The impact assessment methodology

in the Draft Alternative Analysis Guide can become complex due to the large number of hazard traits in the SCP regulations, accessibility of available data, and number of relevant factors to consider. Details for implementation are pending as the State of California Alternative Analysis Guide detailing the methods for deriving the 16 factors is still in draft form.

Baitz et al. [5] advocate a green chemistry method that incorporates a lifecycle approach that includes reducing energy demand, increasing non-fossil resources in energy, increasing non-fossil resources as feedstock, improving product applications, and improving end-of-life routes. However, Baitz et al.'s [5] green chemistry approach does not provide specific guidance on how to measure such improvements nor does it address several of the 12 principles such as atom economy, less hazardous chemical syntheses, and designing safer chemicals.

In addition, GlaxoSmithKline and Merck & Co. [8] have developed approaches to green chemistry. GlaxoSmithKline developed an approach that uses process mass intensity (PMI) and global warming potential to evaluate the lifecycle impacts for new compounds. GlaxoSmithKline's approach is relevant for only one of the 12 principles, namely atom economy. GlaxoSmithKline also developed the Solvent Selection Guide, which compares solvents based on hazard characteristics and a solvent process LCA ranking. While only focused on a specific list of solvents and not all of the materials in the chemical synthesis, the Solvent Selection Guide incorporates indicators for waste prevention, atom economy, less hazardous chemical syntheses, designing safer chemicals, less hazardous chemical synthesis, safer solvents and auxiliaries, design for energy efficiency, and inherently safer chemistry for accident prevention. It does not explicitly include an indicator for use of renewable feed-stocks, though this is potentially included in the waste and lifecycle indicators [9]. GlaxoSmithKline has developed other LCA tools such as a tool to compare synthetic route lifecycle tool does not include waste, solvent recovery, or specific chemical-related health and safety data and does not address all of the 12 principles, omitting for example atom economy and inherently safer chemistry for accident prevention, to name a few [10]. GlaxoSmithKline combined Merck & Co.'s PMI tool with their synthesis routes LCA tool to make a streamlined LCA tool for the pharmaceutical industry; however, the new tool still falls short of addressing the full suite of 12 principles, omitting for example inherently safer chemistry for accident prevention among others [11].

A life cycle assessment (LCA) is a detailed modeling approach that can be used for green chemistry evaluation by quantifying impacts over a product's lifecycle [12]. However, collecting data and completing modeling for a rigorous LCA is a time-consuming activity, and at times representative input data are not readily available [13]. Furthermore, LCA often does not address each of the 12 principles. LCA can be used to investigate specific environmental impacts of a product or process, to compare the impacts between products or processes, and to scrutinize the source of an impact by lifecycle stage or process component

[14]. However, the robustness of LCA results are dependent on a number of factors including the quality and treatment of input data, boundaries selected by the modeler, and the choice of characterization factors [15]. As noted, LCA often omits one or more of the 12 principles. For example, worker safety, a key element of principle 12, is not routinely considered in LCA [16,17]. Methods to create LCA characterization factors for work related exposures are in development, but data quality is limited [16].

Studies indicate that results from LCA may differ from assessments using green design metrics. Tabone et al. [18] evaluated the ability to use the 12 principles to reduce lifecycle environmental impacts of polymers by comparing green design metrics with LCA, specifically for a case study of 12 polymers. The study found that polymers that adhere to green chemistry principles had lower lifecycle environmental impacts. However, results were not uniform; for example, polymers with biological feed-stocks had higher environmental impacts than polymers with petroleum feed-stocks while ranking higher in green design. This disparity is due to the assumption in green design metrics that using renewable resources is desirable (principle 7), contrasted with the complications inherent in evaluating the upstream impacts of biomaterial use. Certain biopolymers showed higher eutrophication, human health, and eco-toxicity impacts from fertilizer use, pesticide use, and land use in agricultural production, as well as fermentation and other chemical processing steps required converting the biomaterial into plastic. However, the fundamental premise of principle 7 is that it is better to use renewable rather than depleting materials, with recognition that with time least impactful measures for deriving renewable materials will be established [19]. Further study comparing results from LCA with this DOZN™ approach may improve the usability and interpretation of the DOZN™.

Rather than adopting a full LCA approach, the Green Chemistry Metric approach (DOZN™) relies on readily available standardized information, applied in a consistent and transparent fashion for purposes of comparing alternatives using a discrete set of widely agreed upon principles. The DOZN™ approach relies on data that meet global industry standards, such as the globally harmonized system of classification and labeling of chemicals (GHS) [20] and standardized boundaries to facilitate transparency and comparability. The DOZN™ approach and LCA serve as complementary approaches. While the DOZN™ approach, by virtue of its focus on the 12 principles, does not include all of the detail of a well-designed LCA, it does facilitate efficient consideration of key principles.

In summary, none of the alternative methods identified offered the combined strategy of using readily available data to comprehensively, transparently, efficiently, and quantitatively evaluate chemical and process alternatives according to all of the 12 principles. The ability to capitalize on readily available data for green chemistry evaluation, as incorporated into this DOZN™ approach, is a relatively recent phenomenon. This availability of data is tied to the timely development, use, and adoption of the

GHS classification system, which provides an influx of information on the physical, health, and environmental hazards of individual chemicals. Additionally, the DOZN™ approach leverages other product specific information to address the full complement of the 12 principles. The DOZN™ approach and scoring method are described herein and demonstrated with a case study.

## Methods

### DOZN™ Approach

The design objectives developed by MilliporeSigma industrial chemists for the DOZN™ included the following: (a) allow for direct comparison between alternative chemicals considered for the same application, as well as direct comparison between alternative synthesis manufacturing processes considered for the same chemical product; (b) allow transparent comparison against each of the 12 principles and for each of the three major stewardship categories: resource efficiency, human health and environmental hazard, and energy use; (c) provide sufficient flexibility to apply to the diverse product portfolio; (d) be inexpensive to implement by utilizing readily available data; (e) be based on generally accepted industry practices, when available; and (f) be easy to communicate the method and results to customers. Considering these guiding elements, we investigated and designed a best approach to evaluate and score chemical products and processes on each of the 12 principles.

### Framework for Scoring and Ranking Chemicals and Processes by DOZN™

The DOZN™ approach incorporates principle-specific algorithms to compare and rank chemical and process alternatives under consideration. The approach is to calculate a principle score (PS) for each of the 12 principles (PS 1–12) using chemical specific data readily available from a number of sources, including that of Globally Harmonized System. The PSs metrics are key for development of comparison and ranking strategies and, as such, contribute to the flexibility of the DOZN™ approach.

Principle-specific scores (e.g., PS-1) can be used for the assessment of alternative performance under individual GC principles. In other words, PS-1 values from alternatives can be compared; PS-2 values can be compared, and so on. Because chemical-specific PS are based on different end points and therefore different measurement scales, aggregate scores calculated by direct summation of individual PSs would disproportionately represent metrics with higher possible scores. Therefore, ranking strategies were developed to avoid the uncertainty and controversy associated with data conversions to a common scale.

Ranking strategies for assessment of alternatives under DOZN™ are based on a hierarchy of metrics based on individual principles, categories of principles, and a summation of all 12 principles. Elements of this hierarchy are described as follows.

### Individual GC Principles

Each principle-specific score (PS 1–12) is assigned a rank of 1-to-n (where n is the number of alternatives being compared)

to derive the principle-specific score rank score (PSR 1–12). For example, when comparing three product alternatives on principle 1, the principle scores are ranked 1, 2, and 3 to derive principle specific rank scores of PSR 1–1, PSR 1–2, and PSR 1–3. These principle specific rank scores can then be considered together to rank alternatives by category, or across the full spectrum of 12 principles.

### Categories

The DOZN™ also groups the 12 principles into like categories, allowing for a focus on overarching green chemistry categories of hazard, resource use, and energy efficiency. These category groupings are shown in Table 1: improved resource use, increased energy efficiency, and reduced human and environmental hazards.

Improved Resource Use	Increased Energy Efficiency	Reduced Human and Environmental Hazards
Principle 1: Waste prevention	Principle 6: Design for energy efficiency	Principle 3: Less hazardous chemical synthesis
Principle 2: Atom economy		Principle 4: Designing safer chemicals
Principle 7: Use of renewable feedstock		Principle 5: Safer solvents and auxiliaries
Principle 8: Reduce derivatives		Principle 10: Design for degradation
Principle 9: Catalysis		Principle 12: Inherently safer chemistry for accident prevention
Principle 11: Real-time analysis for pollution prevention		

**Table 1:** 12 Principles Categories.

The category rank (CR) is determined by ranking the average of PSRs in that category. For example, the CR for improved resource use is determined by ranking the average of the PSRs for principles 1, 2, 7, 8, 9, and 11 for each alternative. If five alternative chemicals are being compared, therefore, there will be category rankings of 1–5 for each category. It is important to note that while in some cases a principle may contribute to the environmental benefits of more than one category, this method group's principle into those categories where benefit is most relevant.

### Summary of All Principles

To allow the user to consider all 12 principles in comparisons of chemical products or processes, the DOZN™ uses a summary rank (SR). The SR is the rank for each alternative of the average of all 12 PSRs.

### Approach to Leverage Readily Available Data

Given the breadth of global and U.S. agency adoption of the GHS, aligning the DOZN™ with and using GHS data, where relevant, presents the best opportunity for integrating readily available data into the method. GHS data are relevant to most of the principles (principle 3, 4, 5, 10, and 12) encompassed in the reduced human and environmental hazards category. For example, for those principles related to health hazards, i.e., 3, 4, and 5, the DOZN™ considers a

combination of GHS toxicity ratings by exposure route across end points to assign a relevant PS. Relevant GHS health hazard criteria include those applicable to acute toxicity, skin corrosion/irritation, serious eye damage/eye irritation, respiratory or skin sensitization, aspiration toxicity, reproductive toxicology, target organ systemic toxicity (single and repeated exposure), germ cell mutagenicity, and carcinogenicity. Similarly, GHS-based classifications for environmental hazards and physical hazards are useful to scoring principles 10 and 12, respectively. Specifically, principle 10 uses GHS-derived information on environmental hazard criteria (e.g., acute aquatic toxicity) and biodegradation, and principle 12 uses a combined consideration of the 16 GHS-defined physical hazard categories (e.g., explosives, flammable gases, flammable aerosols, and oxidizing gases).

In addition to the GHS, the DOZN™ uses readily available information to represent other metrics such as energy use or waste generation. Such information may be a direct measurement or proxy data, such as time in various heating or cooling conditions to represent metrics, such as energy use.

### Flexibility with Lifecycle Stages

When using the DOZN™ scoring method, boundaries must be established to ensure that the same lifecycle stages—such as raw materials extraction, raw materials preprocessing, chemical manufacturing, or disposal are equally included or excluded from each of the chemicals or processes being compared. If the boundaries exclude a particular lifecycle stage, then whichever of the 12 principles require that lifecycle stage must also be excluded. For transparency, such exclusions and reasons for exclusions should be specified. For example, if three chemicals are to be compared and only one chemical has data for an applicable lifecycle stage, then that lifecycle stage and principles applicable to that lifecycle stage should be transparently excluded for all three chemicals.

Further detail on the approach selected for computation of each principle specific green chemistry metric is presented below.

### Results

Using the DOZN™ approach described above, principle-specific algorithms (P- DOZN™) were developed to guide calculation of each of the 12 PS and associated rankings. For each of the three DOZN™ categories, as shown in Table 1, we describe the principles included in that category, their P- DOZN™, and the complementary nature of the principles in the category. We describe herein the parameters engaged to develop the algorithm and basic approach.

### Improved Resource Use Category

The improved resource use category includes the principles that drive resource efficiency and waste reduction (Table 1). This collection of principles addresses resource use in a variety of manners. Principle 1 and principle 2 drive an overall approach to resource efficiency by considering the relationship between input materials and the desired product produced. The algorithm for calculating the PS for principle 1 (P1- DOZN™) focuses on

managing waste with an eye toward waste hazards by including a waste severity factor. The P2- DOZN™ complements the P1- DOZN™ by focusing on the efficient use of inputs, rather than waste. Principle 76 and the accompanying P7- DOZN™ focus on resource efficiency to the extent that renewable materials are used as inputs. P8- DOZN™, P9- DOZN™, and P11- DOZN™ address resource efficiency in the manufacturing process through reduction in derivatization waste, increased use of catalyst, and use of more careful monitoring, respectively.

### Application of DOZN™

The DOZN™ approach allows transparent comparison between chemicals based on each of the 12 principles. The DOZN™ scoring method was designed to optimize transparency and clarity of communication. Fundamental to the scoring method is that, first, companies define equivalent boundaries of comparison and, second, the scoring method defines a hierarchy of metrics including principle score rank (PSR), category rank (CR), and summary rank (SR) to allow multiple chemical products or synthetic manufacturing processes to be compared. As the DOZN™ have been designed such that a lower PS represents a greener option, the principle with a lowest PS will be assigned a PSR of 1 and the principle with a higher PS will be assigned a PSR of 2 etc. If the PSR averages are tied, then the two alternatives receive the same rank. The mean of PSRs by category are then ranked to determine CR, category rank, and the mean of PSRs for all 12 principles are then ranked to determine SR, summary rank. Ranking each chemical for each PS allows users to transparently see in what manner chemicals or chemical processes improve green chemistry over alternatives, as well as where there are trade-offs between green chemistry principles.

### Case Study

MilliporeSigma industrial chemists trialed the DOZN™ in a case study and found that the DOZN™ provided for the ability to evaluate and score chemical products and processes on each of the 12 principles and met the key design objectives delineated above. This case study compares two alternative processes an original and a re-engineered process to synthesize 1-aminobenzotriazole to evaluate and score the greener alternative using the DOZN™ approach. The original process to synthesize 1-aminobenzotriazole includes four steps illustrated. The second step includes a hazardous hydrogenation step at atmospheric pressure using 10% palladium/carbon in methanol (20 L flask). The final product is purified by silica gel column using kilograms of silica gel and additional tens of liters of organic solvents. The re-engineered process solves this problem as it does not need column purification.

The new process to synthesize 1-aminobenzotriazole is a one step process illustrated in Figure 2. The nucleophilic reaction of benzotriazole with hydroxylamine-O-sulfonic acid in alkaline aqueous solution gives 1-aminobenzotriazole. The final product is purified by extractions, washings, and recrystallization.

Some of the improvements of the re-engineered process include the following: the hazardous hydrogenation procedure at atmospheric

pressure using 10% palladium/carbon in methanol (20 L flask) was eliminated from the process, 40% less organic solvents, eliminated about 6 L of concentrated hydrochloric acid and 150 g of 10% palladium/carbon catalyst waste disposal, used 6 kg less auxiliaries (e.g., sodium acetate/carbonate/sulfate), reduced 22 days (73%) process time, and product yield was increased by about 60%.

On the basis of the improvements, the original and redesigned alternatives were compared based on each of the 12 P- DOZN™. They were then scored by ranks by principle and by category. The alternatives were compared with the following boundary setting assumptions: The lifecycle stage included in the case study boundaries is chemical manufacturing. The case study excludes raw materials extraction, raw materials preprocessing, and disposal. These lifecycle stages are excluded to provide a simplified example. The case study boundaries did not include any raw material inputs or intermediates.

Table 2 provides the results of the greener alternative example. The results table is organized to compare chemicals scores and ranks by principle and by category. In this example, the re-engineered 1-aminobenzotriazole process only ranks better (has a lower PSR) than the original 1-aminobenzotriazole process for principles 1–3, 5–7, and 12. The re-engineered 1-aminobenzotriazole process ranks better (has lower CRs) in all three categories, and the re-engineered 1-aminobenzotriazole process is better overall (has an improved SR) compared to the original 1-aminobenzotriazole process. The DOZN™ provides directional evidence that the re-engineered process is better or the same in 11 out of 12 principles (only worse for principle 9), all three categories, and overall. Ultimately, the end user will decide if they will prioritize chemical selection based on individual principles, categories, or an overall rank. This case study and the DOZN™ method were not peer reviewed by other industrial chemists outside of MilliporeSigma, which is a potential limitation of this research.

The DOZN™ is advantageous over existing approaches, because it provides metrics that are (i) inexpensive to implement with readily available data, (ii) based on generally accepted industry practices when available, and (iii) an easy way to communicate the method equations and results to customers. Sustainability programs that implement the proposed approach should anticipate the following benefits:

- **Measurement:** ability to use on-hand data sources or establish straightforward data collection programs
- **Calculations:** ability to utilize well-defined metrics to calculate the benefits of the 12 principles of green chemistry
- **Communication:** ability to transparently communicate greener alternatives to customers

As with all methods, including those as established as LCA, there are limitations. We propose the following next steps to improve upon this research:

- Engage a green chemistry working group to pilot and review the method

- Conduct an LCA to compare the DOZN™ results with LCA results

Considering these guiding elements, we investigated and designed an approach to evaluate and score chemical products and processes on each of the 12 principles.

More information related to DOZN™ can be found at <http://www.sigmaaldrich.com/greener>.

Category and Related Principles	Old 1-Aminobenzotriazole Process	Re-engineered – 1-Aminobenzotriazole Process
	Principle Score	Principle Score
<b>Improved Resource Use</b>		
Principle 1: Prevent Waste	2701	1042
Principle 2: Atom Economy	933	345
Principle 7: Use of Renewable Feedstock	933	345
Principle 8: Reduce Derivatives	0.0	0.0
Principle 9: Catalysis (vs. Stoichiometric)	0.5	1.0
Principle 11: Real-Time Analysis for Pollution Prevention	1.0	1.0
<b>Increased Energy Efficiency</b>		
Principle 6: Design for Energy Efficiency	3282	1322
<b>Reduced Human and Environmental Hazards</b>		
Principle 3: Less Hazardous Synthesis	3358	1455
Principle 4: Design Benign Chemicals	5.0	5.0
Principle 5: Benign Solvents and Auxiliaries	2245	1252
Principle 10: Design for Degradation	0.0	0.0
Principle 12: Inherently Benign Chemistry for Accident Prevention	2516	220
Aggregate Score*	100	44

**Table 2:** Greener Alternatives Example.

\*Aggregate Score is calculated by averaging each category scores, and summing three category scores to get the single score. Then this will be further normalized (divided by 50) to get an aggregate score from 0 to 100 scales (0 being the most desired).

## Conclusions

The DOZN™ is advantageous over existing approaches, because it provides metrics that are (a) inexpensive to implement with readily available data, (b) based on generally accepted industry practices when available and (c) easy to communicate the method and results to customers. Sustainability programs that implement the proposed approach should anticipate the following benefits:

- Measurement:** Ability to use on-hand data sources or establish straightforward data collection programs.
- Calculations:** Ability to utilize well-defined metrics to

calculate the benefits of the 12 principles of green chemistry.

- Communication:** Ability to transparently communicate greener alternatives to customers.

Based on the feed-back from customers, MilliporeSigma is currently working on expanding DOZN™ system to DOZN™ 2.0, so customers can screen their products/processes to get DOZN™ scores. This would help our customers to select the greener products for their research/manufacturing to promote sustainability.

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