Section I — Assessing Chemicals

8. PURPOSE

Section I outlines the procedure to perform a GreenScreen assessment of a chemical compound (also referred to as “chemical” or “compound”), either organic or inorganic, including how to assess and classify hazards and assign a GreenScreen Benchmark™ score.

8.1 A GreenScreen assessment of a chemical includes a comprehensive review of all available information including 1) measured data from toxicological studies in the scientific literature, 2) estimated data from suitable analogs and models, and 3) hazard lists.

8.2 GreenScreen Specified Lists™ are the hazard lists required to be searched for a GreenScreen assessment. The GreenScreen Specified Lists are included in the GreenScreen Chemical Hazard Criteria in Annex 1 and the GreenScreen List Translator Map in Annex 12. Licensed GreenScreen List Translator Automators provide tools to search all GreenScreen Specified Lists efficiently.

9. SCOPE

9.1 The procedure below must be used to derive a Benchmark score for a chemical compound. Assessors must apply expert judgment when evaluating appropriateness of available toxicological data for classifying hazards of the chemical compound, including consideration of varying concentrations of impurities in experimental test substances.

9.3 See Section II for polymers.

9.3 See Section III for products.

10. PROCESS OVERVIEW

The following figure illustrates the relationship between GreenScreen resources in the Annexes and the various steps performed in conducting a GreenScreen assessment of a chemical. The order of steps may vary based on individual preference.
SECTION I — ASSESSING CHEMICALS

FIGURE 1. GreenScreen Chemical Assessment Procedure

<table>
<thead>
<tr>
<th>Assess and Classify Hazards</th>
<th>Assign a Benchmark Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>STEP 1 – IDENTIFY CHEMICAL TO ASSESS</td>
<td>STEP 6 – ASSIGN A GREENSCREEN BENCHMARK™ SCORE</td>
</tr>
<tr>
<td>STEP 2 – RESEARCH</td>
<td></td>
</tr>
<tr>
<td>Step 2a – Conduct a comprehensive data review. You can use Information Sources (Annex 10) to start</td>
<td>Step 6a – Determine the preliminary Benchmark score using the Benchmark Criteria for Organic or Inorganic Chemicals (Annex 3 or 4) and the Benchmark Worksheet (Annex 6)</td>
</tr>
<tr>
<td>Step 2c and 2d – Use estimation (i.e. analogs and models) to fill in for missing measured data</td>
<td>Step 6c – Document Benchmark results in a Chemical Assessment Report Template</td>
</tr>
<tr>
<td>Step 3a – Classify hazard level for each of the 18 hazard endpoints using Chemical Hazard Criteria (Annex 1) and Hazard Endpoint Classification Guidance (Annex 2)</td>
<td></td>
</tr>
<tr>
<td>Step 3b – Determine level of confidence for each hazard</td>
<td></td>
</tr>
<tr>
<td>Step 3c – Assign a data gap to each hazard endpoint with insufficient information</td>
<td></td>
</tr>
<tr>
<td>Step 3d and 3e – Document results in a Chemical Assessment Report (Section VI – Template 1)</td>
<td></td>
</tr>
<tr>
<td>Step 4 – IDENTIFY ENVIRONMENTAL TRANSFORMATION PRODUCT(S)</td>
<td></td>
</tr>
<tr>
<td>See Transformation Product Resources and Worksheet (Annex 9)</td>
<td></td>
</tr>
<tr>
<td>STEP 5 – ASSESS ENVIRONMENTAL TRANSFORMATION PRODUCTS</td>
<td></td>
</tr>
</tbody>
</table>

Copyright © (2014–2018) by Clean Production Action, All rights reserved. No part of this publication is to be reproduced or utilized in any form or by any means, without prior written permission from Clean Production Action.
11. ORGANIC CHEMICAL ASSESSMENT PROCEDURE

This sub-section 11 describes the assessment and classification procedure for an organic chemical. This sub-section 11 in combination with sub-section 12 describes the chemical assessment and classification procedure for an inorganic chemical.

11.1 Step 1 – Identify Chemical to Assess

Determine the chemical compound to be evaluated and report the chemical abstract service number (CASRN) and chemical structure.

If a GreenScreen assessment specific to a particular manufacturer and trade name is desired, then the assessor must follow the procedure outlined in Section III for a chemical substance.

11.2 Step 2 – Research

Assessing chemicals is accomplished by examining comprehensive toxicological data, checking GreenScreen Specified Lists, and using estimated data from suitable analogs or modeled data where measured data are lacking for the parent chemical. A “strength of evidence” approach may be used and the rationale behind the hazard classification should be clearly stated, particularly in the case where multiple studies are available that measure the same hazard endpoint. The order of steps may vary based on individual preference (e.g., reviewing Specified Lists prior to conducting a toxicological review).

11.2.1 Step 2a – Conduct a comprehensive data review

Review all available measured data from standardized tests and scientific literature:

1) Primary literature sources, authoritative secondary sources that are peer reviewed, and authoritative sources are preferred. Examples of peer reviewed authoritative secondary sources include IARC Monographs, government risk assessments, and authoritative toxicology databases.

2) Other high quality secondary sources are acceptable.

a. If a study is cited from a secondary source, it must be referenced as a secondary source.

b. Publicly available primary data for Flammability and Reactivity may not be available. Secondary sources such as Safety Data Sheets (SDS) may be used for Flammability and Reactivity when there are no other options.

11.2.2 Step 2b – Review all GreenScreen Specified Lists

1) When conducting GreenScreen assessments, it is mandatory to search all GreenScreen Specified Lists and report the results. Third parties have developed automated software to assist with searching; see Section IV for comprehensive guidance on performing a GreenScreen List Translator assessment.

2) To classify hazards, use the information contained within the GreenScreen Specified Lists in combination with the literature review and expert judgment.

3) See Section IV for a description of how GreenScreen Specified Lists are categorized (i.e., Authoritative A or B, and Screening A or B).

11.2.3 Step 2c – Use measured data from suitable analog(s) to fill missing data

1) Provide information on whether and why a suitable analog(s) was used to evaluate one or more hazard endpoints that were missing measured data. If a suitable analog(s) was not used, include rationale in the final report for not using one or more of the...
analogs identified. A suitable analog is a chemical that shares similarities in structure, function and mechanism of action with the chemical being assessed. In some cases, the analog may be a metabolite or transformation product. Examples of resources to identify analogs and guidance for using analogs are provided in number 3 (a-g) below.

2) For each suitable analog used, provide the name and chemical structure, the applicable hazard endpoint(s), and the rationale for why it is considered suitable for each of the hazard endpoint(s). Suitable analog selection is hazard endpoint/parameter dependent, and the choice can be different for different endpoints.

3) Profilers and Practitioners must make a good faith effort to review at least one readily available suitable analog for each hazard endpoint missing data for the parent chemical and consult at least one of the following publicly accessible tools. While beyond the minimum requirements, additional suitable analog identification and assessment may be performed and may add to the quality of the assessment.

   c) REACH dossiers (Registration, Evaluation Authorisation and Restriction of Chemicals) (http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances, accessed 9/18/17);
   d) High Production Volume Information System (HPVIS) (https://ofmext.epa.gov/HPVISlogon, accessed 9/18/17);
   f) Environmental Protection Agency (EPA) chemical categories (from New Chemicals program) (https://www.epa.gov/reviewing-new-chemicals-under-toxic-substances-control-act-tsca, accessed 9/18/17); and/or
   g) Other risk assessment/risk management regulatory or government documents.

11.2.4 Step 2d – Use estimated data from a model to fill in missing measured data

At a minimum, use the Sustainable Futures suite of models (1-3 below). These models use quantitative structure activity relationship (QSAR) methods to apply statistical tools correlating biological activity of chemicals with descriptors representative of molecular structure and/or properties.

   1) EPISUITE: Software containing physical/chemical property and environmental fate estimation programs. (https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface, accessed 9/18/17);
   2) ECOSAR: The Ecological Structure Activity Relationships (ECOSAR) Class Program estimates the acute and chronic aquatic toxicity of industrial chemicals. (https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model, accessed 9/18/17); and/or

4) While beyond the minimum requirements, additional models may also be useful and enhance the quality of the assessment (e.g., OECD Toolbox at http://www.oecd.org/chemicalsafety/risk-assessment/oecd-qsar-toolbox.htm, accessed 9/18/17).

11.3 Step 3 – Classify Hazards

11.3.1 Step 3a – Classify hazard level for each hazard endpoint

1) The GreenScreen Chemical Hazard Criteria in Annex 1 are used to classify the hazard level for the parent chemical as High (H), Moderate (M), Low (L) or in some cases very High (vH) or very Low (vL) for each hazard endpoint. The same criteria are used to evaluate any feasible and relevant environmental transformation product(s) as outlined in sub-section 11.4 and 11.5. Figure 2 depicts the GreenScreen Chemical Hazard Criteria for Carcinogenicity, as an example.

2) Evaluate data for all relevant routes of exposure. Always consider data for oral, dermal, and inhalation routes of exposures when available. Consider other routes of exposure on a case-by-case basis only (e.g., transplacental transport, lactational transfer, intraperitoneal or subcutaneous injection).

3) In reviews that include conflicting data, use a “strength of evidence” evaluation aimed at the protection of human health and environment to inform the hazard designation. There are a number of resources for reporting strength of evidence (e.g., ECHA Practical Guide 2 – How to report weight of evidence; https://echa.europa.eu/support/registration/how-to-avoid-unnecessary-testing-on-animals/weight-of-evidence, accessed 12/15/17).

4) All data are considered in the assessment, unless there is a very strong scientific rationale to discount a study. Especially with emerging science, there may be disagreement about some studies and/or hazard classifications. Clear and detailed rationale needs to be articulated in the assessment report in order to discount a study.

5) A structural alert can be used as a line of evidence to classify a chemical as Moderate, High, or very High hazard. However, lack of a structural alert alone is not sufficient to classify the chemical as Low hazard. In some cases, sufficient negative data can be used to assign a Low hazard despite the existence of a structural alert. In those cases, the assessment must note the presence of the specific structural alert(s) and provide rationale for assigning a Low hazard in the presence of any structural alert(s).

6) For more in-depth guidance on classifying the hazard level for Reproductive and Developmental Toxicity, Endocrine Activity and Systemic Toxicity, see Annex 2.
11.3.2 Step 3b – Determine level of confidence (high or low) for each hazard level assigned

Level of confidence is determined by data source(s), data quality, and expert judgment considering the strength of evidence. The rationale behind the assigned level of confidence must be provided for each hazard endpoint.

1) Determine confidence level of each study, listing, or estimation. Measured data, estimated data, and lists may be considered either high confidence or low confidence data sources.

a. High confidence data sources may include:

i. Presence on an Authoritative A list;

ii. High quality measured data for the chemical being assessed;

iii. High quality measured data for a strong analog.

<table>
<thead>
<tr>
<th>Information Type</th>
<th>Information Source</th>
<th>List Type</th>
<th>High (H)</th>
<th>Moderate (M)</th>
<th>Low (L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data</td>
<td>GHS Criteria &amp; Guidance</td>
<td>GHS Category 1A (Known) or 1B (Presumed) for any route of exposure</td>
<td>GHS Category 2 (Suspected) for any route of exposure or limited or marginal evidence of carcinogenicity in animals</td>
<td>- Adequate data available and negative studies; and - GHS not classified</td>
<td></td>
</tr>
</tbody>
</table>

A Lists

|----------------------------------|---------------|---------------------|---------|---------|


| EU – REACH Annex XVII CMRs | Authoritative | Category 1 or 2 | Category 3 | |
| EU – Annex VI CMRs | Authoritative | Carc 1A or 1B | Carc 2 | |
| EU – GHS (H-Statements) | Authoritative | H350 or H350i | H351 | |
| EU – R-Phrases1 | Authoritative | R45 or R49 | R40 | |
| EU – SVHC Candidate List | Authoritative | Carcinogenic – Candidate list | | |
| EU – SVHC Prioritisation List | Authoritative | Carcinogenic – Prioritized for listing | | |
| EU – SVHC Authorisation List | Authoritative | Carcinogenic – Banned unless Authorised | | |

GHS – (COUNTRY) Lists (Australia, Indonesia, Japan, Korea, Malaysia, Taiwan and Thailand)

<table>
<thead>
<tr>
<th>GHS – [COUNTRY] Screening</th>
<th>Category 1A or 1B or H350 or H350i</th>
<th>Category 2 or H351</th>
<th>Not Classified</th>
<th></th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>IARC</th>
<th>Authoritative</th>
<th>Group 1 or 2a</th>
<th>Group 2b</th>
<th>Group 4</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>MAK</th>
<th>Authoritative</th>
<th>Carcinogen Group 1 or 2</th>
<th>Carcinogen Group 3A or 3B or 4 or 5</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>US CDC – Occupational Carcinogens</td>
<td>Authoritative</td>
<td>Occupational Carcinogen</td>
<td></td>
<td></td>
</tr>
<tr>
<td>US NIH – Report on Carcinogens</td>
<td>Authoritative</td>
<td>Known or Reasonably Anticipated</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CA EPA – Prop 65</td>
<td>Authoritative</td>
<td>Carcinogen</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

B Lists

|----------------------------------|---------------|---------|---|

|----------------------------------|---------------|--------------------------|---|

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>IARC</td>
<td>Authoritative</td>
<td>Group 3</td>
<td></td>
</tr>
<tr>
<td>CA EPA – Prop 65 (with qualifications)2</td>
<td>Authoritative</td>
<td>Carcinogen – specific to chemical form or exposure route</td>
<td></td>
</tr>
</tbody>
</table>
b. Low confidence data sources may include:
   i. Measured data
      1. A study with equivocal results (e.g., effect is not significantly different
         than control when doses are below differentiating GHS criteria levels);
      2. A study that is assigned a low reliability using a rating system such
         as Klimisch scores (e.g., Klimisch scores of 3 or 4);\(^4\)
      3. A study that did not follow Good Laboratory Practice (GLP) or a specific
         test guideline, or evaluated a non-standard effect;
      4. A study evaluating a route of exposure other than oral, dermal, or
         inhalation (e.g., intravenous, intraperitoneal injections). Other routes
         of exposure may be considered high confidence in specific situations.
   ii. Estimated data
      1. Measured data for a weak analog;
      2. Estimated data from a model on either the parent chemical or a
         suitable analog.
   iii. Lists
      1. Presence on an Authoritative B list;
      2. Presence on a Screening list.

2) Use a “strength of evidence” approach to assign the confidence level for the hazard
   classification. Often the body of evidence on a chemical includes multiple studies
   and/or multiple data types (e.g., lists, measured data, estimated data). Each result
   is considered in relation to all other results and factors such as data type and data
   quality. Expert judgment is required.
   a. Higher priority data sources are weighed more heavily than lower priority data
      sources. GreenScreen prioritizes information as follows:
      i. Valid measured data on the chemical(s) being evaluated are generally
         preferred over other types of information, such as hazard lists or estimated
         values (e.g., suitable analogs or QSAR models).
      ii. Authoritative A lists are preferred over Authoritative B or Screening A or B
         lists. When lists conflict, the most conservative of the authoritative results
         should be used.
      iii. General rules of thumb are as follows:
         1. Classify an endpoint as high confidence if the hazard level was determined
            primarily based on one or more high confidence data sources.
         2. Classify an endpoint as low confidence if the hazard level was determined
            using one or more lower confidence data sources in the absence of
            high confidence data sources.
         3. Classify an endpoint as high confidence when multiple lines of evidence
            lead to the same conclusion.

   and Ecotoxicological Data Regulatory Toxicology and Pharmacology 25:1-5.
4. Classify an endpoint as low confidence when there are multiple studies with mixed results that use comparable methods and are of similar quality.

3) Indicate the level of confidence for each designated hazard level using specified fonts (i.e., BOLD versus ITALICS).
   a. Hazard levels must be represented in **BOLD** capital letters to signify high confidence (e.g., H for High).
   b. Hazard levels must be represented in **ITALIC** capital letters to signify low confidence (e.g., H for High).

**11.3.3 Step 3c – Assign a data gap (DG) to each hazard endpoint with insufficient information**

When assessing chemicals, it is ideal to use a complete set of publicly available data covering all hazard endpoints. In reality, most chemicals have insufficient data to assess and classify all of the hazard endpoints.

1) Assign a data gap to any hazard endpoint where there is insufficient information to assess the hazard using measured data on the parent chemical, measured data on a suitable analog, or estimated data on the parent chemical or suitable analog chemical.

2) Assign a data gap only after all avenues have been explored to fill missing data, including using measured data, estimated data, and expert judgment. Unless all these sources are explored, a data gap cannot be assigned.

3) Use a “blank” if the endpoint has not been assessed or until all options for filling a data gap have been exhausted.

4) If a study is truly inadequate based on expert judgment, then it may be preferable to classify the hazard endpoint as a data gap. However, there is a very high bar to discount studies. Follow guidance in sub-section 11.3.2 to discount one or more studies.

**11.3.4 Step 3d – Document hazard levels**

It is essential to provide detailed documentation of the supporting data and rationale for all hazard levels in an assessment report.

1) GreenScreen Licensed Profilers and Authorized GreenScreen Practitioners must use the current version of the GreenScreen Chemical Assessment Template (See Template 1) for the assessment report.

2) Document each hazard level with a summary paragraph containing a scientifically defensible and logical rationale. Include the following elements in each summary paragraph: 1) hazard level, 2) rationale for hazard level, 3) confidence level, 4) rationale for confidence level.

3) Document all supporting data following the guidelines below:
   a. Indicate results from the review of all GreenScreen Specified Lists. It is assumed that all GreenScreen Specified Lists are searched unless otherwise indicated in the assessment report.
   b. Report a single study only once per hazard endpoint. If a study appears in multiple secondary data sources, these multiple data sources are noted, but the study results should not be reported more than once to avoid giving a false sense of the strength of evidence.
SECTION I — ASSESSING CHEMICALS

11.3.5 Step 3e – Fill in the Hazard Summary Table

The Hazard Summary Table is part of Template 1 – GreenScreen Chemical Assessment Report Template, and is used to assign a Benchmark score.

Fill in the designated hazard level for each hazard endpoint in the respective box of the Hazard Summary Table. An example of a fully populated Hazard Summary Table is shown below in Table 1.

1) Indicate the level of confidence using specified fonts (i.e., BOLD versus ITALIC).

2) Indicate hazard endpoint(s) with insufficient information to classify the hazard level in the Hazard Summary Table using a non-bold, non-italicized, and capitalized “DG” in the respective box.

3) The following color scheme is required for shading the box containing the hazard level for each hazard endpoint:

- nVL = deep green
- nL = light green
- nM = yellow
- nH = red
- nvH = deep red
- DG = white
- Blank = not assessed

4) It is optional to include an additional Hazard Summary Table that shows the hazard level of relevant hazard endpoints by each route of exposure separately. This optional table is provided in the Appendix of Template 1 – GreenScreen Chemical Assessment Report Template.
11.4 Step 4 – Identify Environmental Transformation Product(s)

The GreenScreen Benchmark score for a chemical includes the evaluation of the chemical itself (i.e. parent chemical) and any feasible and relevant environmental transformation product(s) of the parent chemical.

The goal is to identify only those environmental transformation products that are both feasible and relevant because they: 1) are known or likely to form; and 2) are more persistent, bioaccumulative, and/or toxic than the parent chemical.

11.4.1 Identify potential environmental transformation products

The first step is to identify potential environmental transformation product(s) of the parent chemical. Identifying environmental transformation products can be challenging and will require the use of expert judgment. Transformation products for most chemicals are not well studied.

Review literature and other sources for information on known transformation pathways and products.

Note: evaluation of metabolic transformation products is incorporated into the hazard assessment for the parent chemical and is outside of the scope and intention of environmental transformation products and this section.

11.4.2 Determine if feasible

For each environmental transformation product identified, determine whether it is feasible. Then fill in the table in the assessment report template to indicate whether it is feasible or not.

1) Feasible means the transformation product is likely to occur because: 1) the structure of the parent chemical allows for certain types of transformations (e.g., hydrolysis); and 2) those transformations are likely to occur based on the functional use of the chemical across its life cycle (e.g., used in products that are discharged to water).

2) Identification of feasible environmental transformation products will require expert judgment and best available knowledge of the parent chemical’s structure, physical/chemical properties, functional use and partitioning in environmental media.
3) Resources are provided in Annex 9. As a guide, consider the following questions:
   a. Does the parent chemical contain functional groups that can hydrolyze? Oxidize? Photolize? Undergo oxidation or reduction? Are there structural alerts for these transformations? What are the kinetics? The faster the transformation, the more likely that a transformation product will form and result in exposure.
   b. Has the chemical been tested or modelled for biodegradability? Under what conditions? What test methods have been used and what media do they represent (e.g., aerobic freshwater, wastewater treatment, anaerobic biodegradation, marine environment, soil, sediment, etc.)? Is the biodegradation primary or ultimate? What are the kinetics?
   c. Based on the known functional use of the chemical in a product and the life cycle of the product, is the chemical likely to undergo the feasible transformation pathways?
   d. Provide a rationale for the selection and deselection of feasible environmental transformation products.

11.4.3 Determine if relevant

For each feasible environmental transformation product identified, determine if it is also relevant. Then fill in the table in the assessment template to indicate whether it is relevant.

1) Relevant means the transformation product is: 1) persistent enough to be encountered after use or release of the parent chemical; and 2) not a substance necessary for life or commonly formed in the ambient environment.

2) The worksheet provided in Annex 9 can be used as an internal resource for this step, if desired.
   a. Transformation products that are persistent, bioaccumulative, and/or toxic should be considered relevant whether predicted or found in the environment through monitoring (e.g., formation of DDD from DDT). A transformation product is not considered relevant if it is determined by expert judgment to be transient (e.g., an intermediate formed briefly and subsequently degraded, such as during aquatic biodegradation).
   b. Products of ultimate biodegradation/mineralization (i.e., CO₂ and H₂O) are not considered relevant. Transformation products of chemicals that degrade rapidly and completely (i.e., ultimate biodegradation) are unlikely to form persistent biodegradation intermediates and are therefore not considered relevant. This corresponds to meeting criteria for very Low Persistence in GreenScreen (or Low Persistence with expert judgment).
   c. It is helpful to keep in mind when identifying relevant transformation products that GreenScreen assessments are typically used for comparative purposes. Those transformation products that help discriminate between alternative parent chemicals may be considered relevant.
   d. Provide a rationale for the selection and deselection of relevant environmental transformation products.
11.5 **Step 5 – Assess Environmental Transformation Product(s)**

Assess each feasible and relevant environmental transformation product identified in Step 4 above using GreenScreen List Translator (Section IV) at a minimum. It is optional to conduct a GreenScreen assessment of the feasible and relevant environmental transformation product(s) to obtain more comprehensive results. Record the List Translator score or Benchmark score for each feasible and relevant environmental transformation product in the transformation product table in the assessment template.

11.6 **Step 6 – Assign a GreenScreen Benchmark™ Score**

First, assign a preliminary Benchmark score by comparing the completed Hazard Summary Table for the chemical to the organic or inorganic Benchmark Criteria (Annex 3 or 4, respectively). Next, perform a data gap analysis (see sub-section 11.6.2.1). Consider feasible and relevant environmental transformation products (see sub-section 11.6.2.2) to assign a final Benchmark score.

11.6.1 **Step 6a – Determine the preliminary Benchmark score**

GreenScreen Benchmark™ Criteria apply to individual and groups of hazard endpoints. The Benchmark Criteria for Organic Chemicals can be found in Annex 3 and the Benchmark Criteria for Inorganic Chemicals can be found in Annex 4. All criterion statements for Benchmark-1 must be “false” for the chemical of interest in order to proceed to the Benchmark-2 criteria and similarly for Benchmark-3 and Benchmark-4. For a given Benchmark, if any one (or more) criterion statement(s) is “true” for the chemical, the chemical is assigned the Benchmark score of the “true” criterion statement.

As an example for an organic chemical, the following steps outline the procedure for each Benchmark score, and the table provided in Annex 6 can be used as a worksheet, if desired. The “+” in the criterion statements means “AND,” and the abbreviations for hazard endpoints can be found in the Benchmark Criteria (Annex 3 and 4).

1) **Benchmark-1**: Determine if any of the following Benchmark-1 criterion statements (a–e) are true for the chemical being assessed. A Benchmark-1 is established if any one or more Benchmark-1 criterion statements are true. Once a Benchmark-1 score is established, it is not necessary to proceed to Benchmark-2. If all the following criterion statements (a–e) are false for the chemical, proceed to Benchmark-3 criteria.

   a. PBT = High P + High B + [very High T (Ecotoxicity or Group II Human) or High T (Group I or II* Human)]

   b. vPvB = very High P + very High B

   c. vPT = very High P + [very High T (Ecotoxicity or Group II Human) or High T (Group I or II* Human)]

   d. vBT = very High B + [very High T (Ecotoxicity or Group II Human) or High T (Group I or II* Human)]

   e. High T (Group I Human)

2) **Benchmark-2**: Determine if any one or more of the following Benchmark-2 criterion statements are true for the chemical being assessed.

   A Benchmark-2 is established if any one or more Benchmark-2 criterion statements are true. Once a Benchmark-2 score is established, and it is not necessary to proceed to Benchmark-3. If all the following criterion statements (a–g) are false for the chemical, proceed to Benchmark-3 criteria.
SECTION I — ASSESSING CHEMICALS

11.6.2 Step 6b – Determine the final Benchmark score

1) Conduct a Data Gap Analysis

a. Data requirements become more stringent with higher Benchmark scores. With reliable information on a single endpoint, one can confidently assess a chemical and assign a score of Benchmark-1. Additional data are needed to assess a chemical and confidently assign it a higher Benchmark score. The number and type of data gaps must be considered when assigning a Benchmark score to a chemical. Follow the procedure in Annex 5 to determine whether the preliminary Benchmark score will be modified due to lack of sufficient data when assigning a final Benchmark score.

b. When a chemical fails to meet the data requirements for the preliminary Benchmark score, the chemical is assigned a final Benchmark score that is lower than the preliminary Benchmark score (i.e. Benchmark-2 is lower than Benchmark-3), and equal to the Benchmark score of the highest level of data requirements met by the chemical. The final Benchmark score carries a subscript DG to indicate that data gaps are driving the final Benchmark score.

c. When a chemical meets the data requirements for the preliminary Benchmark score, the chemical is assigned a final Benchmark score that is equal to the preliminary Benchmark score.
2) Evaluate Environmental Transformation Products

If a feasible and relevant environmental transformation product is more hazardous than the parent compound, then the GreenScreen List Translator or GreenScreen Benchmark score of the transformation product is used to modify the Benchmark score of the parent compound.

Each feasible and relevant environmental transformation product must be assessed using GreenScreen List Translator (See Section IV), except for cases where the parent chemical is a Benchmark-1. It is optional to conduct a more comprehensive assessment of feasible and relevant environmental transformation products using GreenScreen (Section II or III) instead.

Follow the steps below to determine whether the parent chemical Benchmark score must be modified due to a feasible and relevant environmental transformation product.

a. Using GreenScreen Benchmark score(s) (optional alternative):
   
i. Identify the lowest scoring feasible and relevant environmental transformation product. This is done by reviewing the Benchmark score for each feasible and relevant environmental transformation product and selecting the one with the lowest numerical value (i.e. Benchmark-2 is lower than Benchmark-3).
   
ii. Compare the Benchmark score of the parent chemical to the Benchmark score of the lowest scoring feasible and relevant environmental transformation product and apply the following:

1. If the Benchmark score of the transformation product is lower than the Benchmark score of the parent chemical, then modify the Benchmark score of the parent chemical to the Benchmark score of the transformation product and add a subscript (TP) (e.g., Benchmark-2_{TP}). The subscript (TP) transparently communicates the parent chemical was assigned a higher Benchmark score and the Benchmark score was lowered based on the score of the environmental transformation product. For example, if the parent chemical was assigned a Benchmark score of 2 and the transformation product was assigned a Benchmark score of 1, then the Benchmark score of the parent chemical is modified to Benchmark-1_{TP}.

2. If the Benchmark score of the transformation product is Benchmark-U, then expert judgment should be used to determine whether the parent chemical Benchmark score should be modified.

3. Report the modified Benchmark score and the rationale for the modified Benchmark score in the GreenScreen Benchmark score and Hazard Summary Table section of Template 1 - GreenScreen Chemical Assessment Report Template.
b. Using GreenScreen List Translator score(s) (minimum required):
   Review the List Translator score of each of the feasible and relevant environmental transformation products identified. Then follow the steps below in order.
   i. If one or more feasible and relevant environmental transformation products were assigned a score of LT-1, assign a final Benchmark score of Benchmark-1_{tp} to the parent chemical. If not, proceed.
   ii. If one or more feasible and relevant environmental transformation products were assigned a score of LT-P1, conduct more research for each to determine whether the transformation product is LT-1 or LT-UNK. If after further research, one or more of the feasible and relevant environmental transformation products is determined to be LT-1, assign a final Benchmark score of Benchmark-1_{tp} to the parent chemical. If not, proceed.
   iii. If all feasible and relevant environmental transformation products are assigned a score of either LT-UNK (initially or after further research) or NoGSLT, do not modify the Benchmark score of the parent chemical.

11.6.3 Step 6c – Document the Benchmark score
   Follow all requirements in sub-section 3 and 4 related to documenting a Benchmark score. In addition, the Benchmark score summary paragraph should include the following three elements:

   1) **Benchmark**: Report the final Benchmark score assigned to the parent chemical based on the inherent hazards associated with the chemical and consideration of data gaps and transformation products as comprehensively defined in this documentation:
      a. Scores modified due to data gaps carry a subscript DG (e.g., Benchmark-2_{DG}).
      b. Scores modified due to environmental transformation products carry a subscript TP (e.g., Benchmark 1_{TP}).

   2) **Rationale**: Include detailed rationale for the final Benchmark score assigned:
      a. If known hazards of the chemical are driving the final Benchmark score, include the hazard endpoint(s) and GreenScreen Benchmark criterion(a) driving the score; or
      b. If data gaps are driving the final Benchmark score, include the final Benchmark score assigned, the preliminary Benchmark score assigned, and data gap(s) and data requirements driving the Benchmark score; or
      c. If a transformation product is driving the final Benchmark score, include the final Benchmark score assigned, the preliminary Benchmark score assigned, the identity of the transformation product driving the Benchmark score (i.e. chemical name, CASRN) and the rationale for why it is considered both feasible and relevant.

   3) **Worst-case**: When one or more data gaps are present for the parent chemical, include a worst-case Benchmark score estimate. This is the Benchmark score that would be assigned if all the data gaps were filled with the highest possible hazard level.
12. INORGANIC CHEMICAL ASSESSMENT PROCEDURE

The physical properties of inorganic chemicals are particularly relevant to assessing their inherent hazard and toxicity, such as solubility, bioavailability, and particle size. For example, water solubility can modify the hazard classification of aquatic toxicity, and particle size and shape can determine the potential for a chemical to cause respiratory irritation. Follow the organic chemical assessment procedure in sub-section 11, with the following additions and/or modifications for inorganic chemicals:

12.1 Step 1 – Identify Chemical to Assess

Follow the guidance in sub-section 11 Step 1.

12.2 Step 2 – Research

In addition to following the guidance in sub-section 11 Step 2, research and report the following form and physical chemical properties of the inorganic chemical in Section VI, Template 1 – GreenScreen Chemical Assessment Report Template.

1) Particle size (e.g., silica particles < 10 microns)
2) Structure (e.g., amorphous vs. crystalline)
3) Mobility (e.g., water solubility, volatility)
4) Bioavailability

12.3 Step 3 – Classify Hazards

Follow guidance in sub-section 11 Step 3 for an inorganic chemical or inorganic feasible and relevant environmental transformation product.

In addition to guidance in sub-section 11 Step 6, make sure to include the inorganic reporting section of the template.

Place an asterisk “*” after the hazard level for Persistence in the respective box of the Hazard Summary Table and include a footnote indicating that the chemical is inorganic.

12.4 Step 4 – Identify Environmental Transformation Products

In addition to following the guidance in sub-section 11 Step 4, consider dissociation products, moieties, and valence states as potential environmental transformation products of inorganic chemicals.

12.5 Step 5 – Assess Environmental Transformation Products

Same as organic chemical guidance. Follow guidance in sub-section 11 Step 5.

12.6 Step 6 – Assign a Benchmark Score

12.6.1 For inorganic chemicals, Persistence should not necessarily be considered a negative characteristic – particularly for naturally occurring substances such as minerals and metal oxides. For this reason, the Benchmark Criteria for Inorganic Chemicals in Annex 4 have been modified in comparison to the Benchmark Criteria for Organic Chemicals in Annex 3 so that Persistence is only considered in combination with chronic hazards. Inorganic chemicals that are persistent and for which all hazard endpoints except Persistence are low may achieve Benchmark-4.

12.6.2 For Benchmarks-1, -2, and -3, Persistence is only considered in combination with Group I, Group II*, and Chronic Aquatic Toxicity hazard endpoints. Persistence is not considered in combination with Group II or Acute Aquatic Toxicity hazard endpoints.

12.6.3 Apply the Inorganic Benchmark Criteria in Annex 4 to assign a preliminary Benchmark score, and determine the final Benchmark score using the same procedure as for organic chemicals.