



Chemical Hazard Scorecard User Guide

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Introduction

This guide serves as a set of instructions for using the Berkeley Center for Green Chemistry (BCGC) Chemical Hazard Scorecard. The main purpose of the scorecard is to assess the relative chemical hazards to human and environmental health of both individual chemicals and chemical formulations they comprise. The scorecard is based on the United Nations Globally Harmonized System (GHS) of toxicological endpoints and reconciles and aggregates various existing scoring systems into one score. The Scorecard is an Excel file that can be downloaded here: <https://bcgc.berkeley.edu/our-work/bcgc-chemical-hazard-scorecard>.

The Scorecard was designed initially to rate the human health and environmental hazard of stereolithography (SLA) formulations used in 3D printing; either existing formulations or potential alternative formulations. This development work was funded by the US EPA Pollution Prevention (P2) Program, 2018-2021.

You can perform a five- step comparative hazard analysis, rank individual chemicals of concern and formulations and compute human health, environmental, and overall scores for their target chemicals. Overall scores are represented as a range of values, based on the individual best and worst scores for constituent factors. Formula scores are computed by the percentages of individual components by weight.

In order to use this scorecard, you will need a full list of the chemicals and their CAS numbers, and percentage by weight for each formulation or proposed formulation. To complete the comparative hazard analysis with this scorecard, you will first have to research available hazard data from curated lists such as the Healthy Building Network's Data Commons (pharosproject.net), or peer-reviewed journals. Next, you will convert hazard data from your various sources to BCGC Scorecard hazard scores for each health/environmental endpoint. The Scorecard will auto-populate these scores in most of the subsequent steps.

The Scorecard includes two examples and space for 10 additional formulations with 10 constituent chemicals each. Cells displaying a '0' contain an Excel function that should not be edited for the auto-fill to work. Here we provide detailed instructions for each step.

Step 1: List all chemicals of interest, identify hazard data, convert to hazard scores

- 1.1 List all chemicals associated with the formulation(s) (existing or potential) in the tab entitled “Step 1. Hazard Data by Fn.” Organize chemicals by function / category. Organizing by function may allow users to “mix-and-match” chemicals within formulations to identify alternatives in Step 2.

	A	B	C	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U
				Carcinogen Mutagen Reproductive Developmental Endocrine				Oral, Dermal, Inhalation and Neurotoxicity				Skin and Eye Irritation		Skin and Respiratory Sensitization		Aquatic Toxicity		Bioaccumulation	Persistence	Other Notes
				Carcinogen	Mutagen	Reproductive & Developmental	Endocrine Disruption	Oral Toxicity	Dermal Toxicity	Inhalation Toxicity	Neurotoxicity	Skin Irritation	Eye Irritation	Skin Sensitization	Respiratory Sensitization	Acute Aquatic Toxicity	Chronic Aquatic Toxicity			
2	Function	Chemical Name	CAS #																	
3	Active Species																			
4		Reactive Monomer - Genomer1122	63225-53-6																	
5																				
6		Reactive Oligomer 1 - Ebecryl8210	CAS #2																	
7																				
8		Reactive Oligomer 2 - SR494LM	CAS #3																	
9																				
10		Chemical #4	CAS #4																	
11																				
12		Chemical #5	CAS #5																	
13																				
14		Chemical #6	CAS #6																	
15																				
16		Chemical #7	CAS #7																	
17																				
18		Chemical #8	CAS #8																	
19																				
20		Chemical #9	CAS #9																	
21																				
22		Chemical #10	CAS #10																	
23																				
24		Backbones																		
25		Castor Oil	8001-79-4																	
26																				
27		Chemical	CAS																	
28																				
29																				
30																				
31																				
32																				
33																				
34																				
35																				
36																				
37																				
38																				
39																				

- Note: the Scorecard lists functions related to SLA resin formulations - active species, backbones, photoinitiators, polymer additives (such as UV blockers and colorants), photobase generators, other constituent chemicals (such as functionalizing intermediates) that are present in the formulation, as well as processing chemicals, degradation product chemicals, and important chemical analogues used to fill data gaps. You can edit the functional categories as needed.
- Put the chemical name in column ‘B’ and the CAS number for each chemical in column ‘C’.
 - For molecular analogues, indicate the primary chemical name and CAS number, as well as what the chemical is serving as an analogue for.

- 1.2 Review and assess hazard data for the health and environmental endpoints for each chemical you have listed. Document the corresponding GHS, Cradle2Cradle, and/or GreenScreen data (see Appendix Steps 1-2).

- 1.2.1 List hazard data for each endpoint in Columns F-U.

- Input applicable GHS classifications (PubMed can be a good source of information).
- For endocrine disruption, document the Cradle2Cradle classification.
- For Bioaccumulation, document the Cradle2Cradle classification and/or the bioconcentration factor.

- d. For Persistence, document the biodegradation half-life and the matrix (freshwater, marine water, soil, sediment) in which the test was run, and/or the results of an OECD 301 biodegradation test.
- 1.2.2 List data sources in cells directly below.
- 1.2.3 There is room for additional notes in column V.

1.3 Convert hazard data into scorecard hazard scores. Refer to the first reference tab, entitled “REF. Hazard Data Conversions,” which designates numerical scores associated with the classifications you have filled out. A screenshot of this tab is shown below.

	A	B	C	D
1	Toxicity Endpoint	Classification or Type of Evidence	Numerical Score	
2	Carcinogenicity	GHS Category 1A or 1B	1	
3		GHS Category 2	2	
4		- GHS Not Classified AND Equivocal Evidence (C2C Yellow)	3	
5		- GHS Not Classified AND C2C Grey		
6		GHS Not Classified AND C2C Green	4	
7		No Data are available	DG	
8	Mutagenicity	GHS Category 1A or 1B	1	
9		GHS Category 2	2	
10		GHS Not Classified	3	
11		GHS Not Classified AND C2C Green	4	
12		No Data are available	DG	
13	Reproductive & Developmental Toxicity	GHS Category 1A or 1B	1	
14		GHS Category 2	2	
15		GHS Not Classified for R and/or D AND Equivocal Evidence for R and/or D	3	
16		- GHS Not Classified for R and D		
17		- GHS Not Classified for R and CNP for D	4	
18	- GHS Classification Not Possible for R and Not Classified for D			
19	No data are available.	DG		
20	Endocrine Disruption	C2C Red	1	
21		C2C Yellow	2	
22		-		
23	Oral, Dermal, and Inhalation Toxicity (Mammalian)	C2C Green	4	
24		No data available for classification	DG	
25		GHS Category 1 or 2 for Acute; GHS Category 1 for STOT (Single Exposure) or Category 1 STOT (Repeated Exposure)	1	
26		GHS Category 3 for Acute; GHS Category 2 for STOT (Repeated Exposure)	2	
27		GHS Category 4 for Acute; GHS Category 2 or 3 for STOT (Single Exposure)	3	
28	GHS Category 5 or GHS Not Classified	4		
29	No data available for classification	DG		
30	Neurotoxicity	GHS Category 1 for STOT (Single Exposure) or STOT (Repeated Exposure)	1	
31		GHS Category 2 for STOT (Repeated Exposure)	2	
32		GHS Category 2 or 3 for STOT (Single Exposure)	3	
33		GHS Not Classified	4	
34	No data available for classification	DG		
35	GHS Category 1 (A, B, C)	1		

1.4 Input the numerical scores corresponding to each endpoint for each chemical into the row below. Entering the numbers 1-4 or ‘DG’ will auto-fill with color.

Step 2: List formulations and list hazard scores for each endpoint

- 2.1 Fill in the chemicals and % weight in formula in the tab titled “Step 2. Hazard Rating,” organized by formulation. If a range of wt% is provided (e.g., in an MSDS), we recommend selecting an average value and noting the range in the ‘notes’ column. Make sure that the sum of all wt% values is 100 for each formulation.
- 2.2 Copy the hazard rating cells from “Step 1. Hazard Data by Fn” for each chemical in the formulation.
- 2.3 Eliminate showstoppers (formulations with extreme hazard).

- a. Showstoppers may either be eliminated from further testing or assigned an overall score of “1” with zero uncertainty.
- b. Any formulation containing any chemicals in concentrations stipulated on the C2CPII Restricted Substances List are considered extremely hazardous. Cross-check whether formulations contain any chemicals on these lists, linked here: <https://www.c2ccertified.org/resources/detail/cradle-to-cradle-certified-restricted-substances-list-rsl>. (Also indicated when using Pharos). We recommend removing any such formulations from further consideration. Note that there may be a limited number of exceptions where chemicals on the RSL could be acceptable for use based on comprehensive hazard assessments.
- c. Any formulation containing any chemical that exceeds 0.1 wt% and is scored a ‘1’ in CMRDE or chronic aquatic toxicity (Step 2) is considered extremely hazardous. We recommend removing any such formulations from further consideration.

Step 3: Roll-up Human Health Group Score

- 3.1 Navigate to tab “Step 3. Human Health Score.” Convert the human health hazard scores to hazard group ratings, each of which is represented as a range from ‘worst’ to ‘best’ using the decision trees for each hazard group, included at the bottom of the scorecard and in Appendix of this guide.
 - a. The chemical names and percentages should auto-fill from Step 2 (shaded in gray).
 - b. Fill in columns D-K manually based on the decision trees.
 - c. The overall human health score for each chemical and for the entire formulation will auto-calculate based on the scores you filled out (columns L-O).

Step 4: Roll-up Environmental Hazard Group Score

- 4.1 Navigate to tab “Step 4. Env Score.” The scorecard will convert environmental hazard scores to an environmental hazard group score for each chemical. The environmental hazard groups are CMR x Fate, Oral/Dermal x Fate, and Aquatic Toxicity x Fate. These toxicity endpoints were selected for environmental hazard in this Scorecard because toxicants acting on these endpoints pose the greatest risk when released into the environment. Fate (persistence and bioaccumulation potential) represents potential exposure when released into the environment.
 - a. For each environmental hazard group, the lowest score is determined for any individual hazard endpoint, where $1 < DG < 2 < 3 < 4$. This value is taken as the ‘Toxicity’ rating for that hazard group (columns F-H). ‘Fate’ is determined by Persistence and Bioaccumulation potential.
 - b. The second reference tab (reproduced in Appendix) is used to determine environmental hazard group scores for each environmental hazard group. The worst case and best case scores will appear in columns I-N.

- c. The overall environment score for each chemical and for the entire formulation will auto-calculate based on the scores generated in columns I-N.

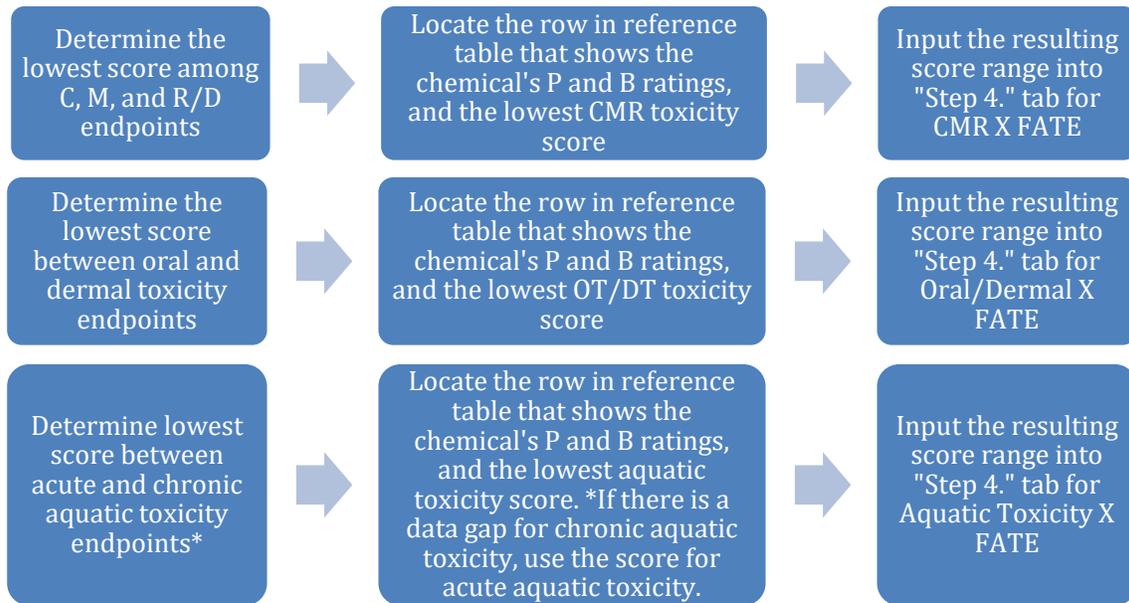
Columns A-H will auto-fill from Step 2.

Columns I-N will auto-fill based on the table in tab "REF Fate x Tox"

1	Entire sheet will auto-fill								Environmental Hazard											
2	Formulation	Chemical in Formulation	% in Material	P	B	Lowest CMR Score	Lowest O/D Score	Lowest Aq Tox Score	Weight: 0.4		0.2		0.4		Worst Case	Best Case	Worst Case	Best Case		
3									CMR X FATE	Oral/Dermal X FATE	Aquatic Toxicity X FATE	Weighted Score per chemical	Weighted Score per chemical	Weighted by % in Material	Weighted by % in Material					
4									Worst	Best	Worst	Best	Worst	Best						
5	PR48	Reactive Monomer - Genomer1122	19.88	4	4	4	4	2	4	4	4	4	4	4	4	4	4	4	4	4
6		Reactive Oligomer 1 - Ebecry8210	39.78	3	4	4	4	2	4	4	4	4	3	3	4	3.6				
7		Reactive Oligomer 2 - SR494LM	39.78	4	4	4	4	2	4	4	4	4	4	4	4	4	4	4	4	4
8		Benetex OB+	0.16	2	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4
9		Igracure TPO	0.4	2	4	DG	4	2	2	4	4	4	4	2	2	3.2	3.83448	3.83768		

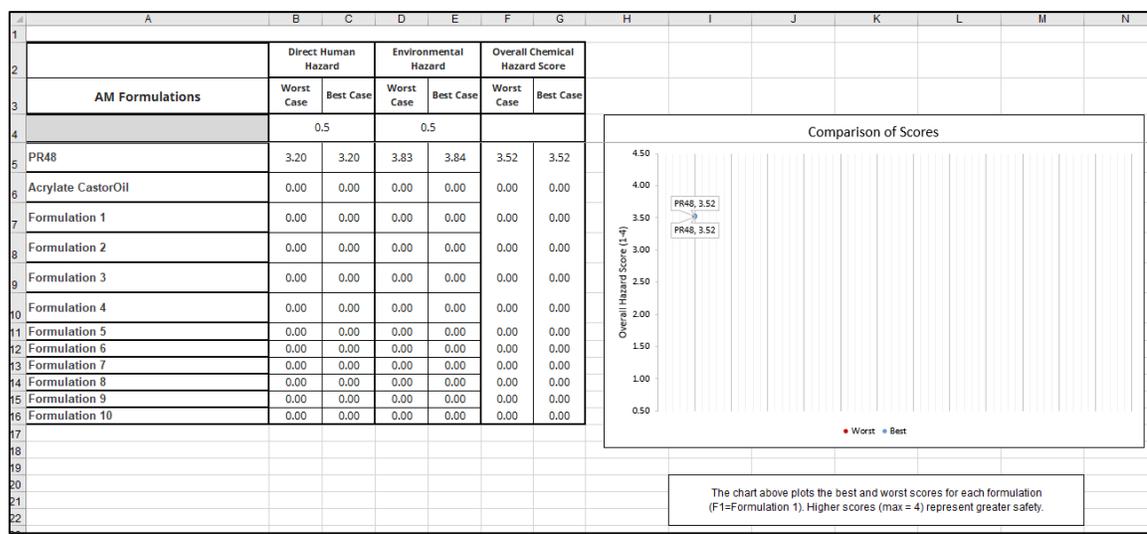
Final scores will auto-calculate based on Columns I-N, weighting in Row 2, and % in Column C

The Scorecard spreadsheet auto-fills with these steps:



Step 5. Review Overall Score Comparisons

- 5.1 The tab titled “Step 5. Overall Score” will auto-fill to provide an overall hazard ranking for all formulations that have been filled in for the previous 5 tabs. See Appendix Step 5 for explanation of the final calculations.
- 5.2 Worst case and best case scores are presented in columns F and G. A visual representation is included as well with the auto-populating scatterplot (higher points represent higher safety). The red points represent the worst case score for that formulation, the blue represents the higher best case score. If the worst and best scores are the same, the blue point will appear.



Optional: Scorecard Customization

Steps 3, 4, and 5 have default values for relative weighting as recommended by BCGC as appropriate for SLA applications. For example, in Step 3, the default weightings reflect the relative health severity of different hazard endpoints. Users may want to change the weightings to reflect the relevance of these endpoints to their context. For instance, the likelihood of exposure via dermal contact may influence the weight attributed to irritation and sensitization endpoints. Formula weightings can be assigned for individual applications/industries informed by industry consensus based on surveys and user testing.

In Step 5, the final formulation scores reflect equal weighting of human health hazard and environmental health hazard. However, users could add columns to account for molecular complexity or non-constituent process chemicals (optionally rated in Steps 1&2) and given weighting coefficients coequal to their estimated impact.