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# Chemical Assessment State of the Science: Evaluation of 32 Decision-Support Tools used to Screen and Prioritize Chemicals

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## ABSTRACT

The last decade has seen an increased focus on evaluating the safety and sustainability of chemicals in consumer and industrial products. In order to effectively and accurately evaluate safety and sustainability, tools are needed to characterize hazard, exposure, and risk pertaining to products and processes. Because many of these tools will be used to identify problematic chemistries, and because many have potential applications in various steps of an alternatives analysis, the limitations and capabilities of available tools should be understood by users so that, ultimately, potential chemical risk is accurately reflected. In our study, we examined 32 chemical characterization tools from government, industry, academia, and non-governmental organizations (NGOs). The tools we studied were diverse, and varied widely in their scope and assessment. As such, they were separated into five categories for comparison: 1) Screening and Prioritization; 2) Database Utilization; 3) Hazard Assessment; 4) Exposure and Risk Assessment; and 5) Certification and Labeling. Each tool was scored based on our weighted set of criteria, and then compared to other tools in the same category. Ten tools received a high score in one or more categories; 24 tools received a medium score in one or more categories, and five tools received a low score in one or more categories. Although some tools were placed into more than one category, no tool encompassed all five of the assessment categories. Though many of the tools evaluated may be useful for providing guidance for hazards – and, in some cases, exposure – few tools characterize risk. To our knowledge, this study is the first to critically evaluate a large set of chemical assessment tools and provide an understanding of their strengths and limitations. *Integr Environ Assess Manag* 2015;11:242–255. © 2014 SETAC.

**Keywords:** Risk assessment Hazard Exposure Tools Chemical alternatives

## INTRODUCTION

Because significant progress has been made in understanding the potential toxicity of existing and new chemicals – as well as their fate, transport, and potential for exposure in the environment – there is an expectation that products must contain chemicals that do not harm people or the environment. Consequently, new regulatory programs, retailer initiatives, and increased public awareness have created enormous pressure on manufacturers and designers to reconsider the chemical ingredients currently used in their products. Many of these programs and initiatives encourage product formulators to embrace the principles of green chemistry, which is defined as designing products and processes in order to minimize use and generation of hazardous substances (USEPA 2014).

A landmark regulation in Europe called the Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) has redefined the manner in which chemicals are approved for use. REACH is a comprehensive risk assessment regulatory framework developed to control chemical exposures and to make accurate and consistent data on the potential hazards of chemicals available to all (Forth and Hayes 2008; Petry et al. 2006). Under REACH, the "burden of proof" falls upon a chemical manufacturer. Chemical manufacturers in the European marketplace must demonstrate that any risk posed to humans or the environment from a chemical they would like to sell, or already sell, can be managed (ECHA 2014). Generally, the chemical registration process entails responsible parties creating chemical-specific dossiers containing information on a chemical's hazard and exposure potential.

Outside of Europe, chemical regulatory reform has been prioritized (e.g., Canada's Chemicals Management Plan) or has been slow to develop (e.g., United States Toxic Substances Control Act reform) and, as such, a patchwork of local mandates, supply chain restrictions, and retailer requirements have filled the void. Nonetheless, all of the regulatory and non-regulatory initiatives have the common goal of eliminating hazardous chemicals in consumer products.

Occupational health scientists have long viewed chemical elimination and substitution as the first steps in controlling chemical exposures to workers (Brandt 1947). The overall goal

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of substitution is to replace currently used chemicals with less hazardous ones, while maintaining the original chemical's effectiveness. For example, in the 1950s, beta-naphthylamine (BNA) was eliminated and substituted with a non-carcinogenic agent as an antioxidant in the rubber industry to reduce the risk of bladder cancer in rubber workers (Veys 1981). Similarly, glass grit has been substituted for sand in abrasive blasting operations in order to eliminate the crystalline silica hazard for workers (KTA-Tator 1998).

While early efforts at chemical substitution in the workplace were focused on identifying replacement chemicals with higher allowable occupational exposure levels (i.e., TLVs, PELs), more sophisticated tools were eventually developed to provide industrial hygienists with a means of using the broader knowledge of a chemical's properties to compare the potential health risks of possible substitutes (Keil 2000). Similarly, concern over ambient air quality, indoor air quality in residential and commercial buildings, chemical registration and product stewardship, contaminated site clean-ups, and pesticide registrations spawned a set of chemical assessment tools developed by the US Environmental Protection Agency (USEPA) and various trade associations. Table 1 lists some of the early tools developed to understand potential chemical exposure.

Although the responsibility of chemical assessment was previously assigned to various governmental agencies (e.g., USEPA, and Food and Drug Administration [FDA]), the era of manufacturer and producer responsibility has been ushered in through regulatory programs such as REACH, many US state regulations, such as California's Safer Consumer Product Act, and voluntary initiatives to obtain 'green' certifications that help differentiate products in the marketplace (e.g., USEPA's Design for the Environment; Eco-Logo). As such, the demand for chemical assessment tools has grown beyond only scientists in government and the chemical manufacturing sector.

To assist product manufacturers with navigating the diverse expectations of the marketplace, many tools have become available that purport to aid in determining the acceptability of a chemical ingredient. The tools are highly varied in their scope, and thus also vary widely in their utility in making chemical selection decisions. In this paper, we present the results of an analysis of 32 decision-support tools used to screen and prioritize chemicals in order to evaluate their safety and sustainability. Our assessment focused on the purpose, functionality, and usefulness of each tool at assessing chemical hazard, exposure, and risk. A discussion of our unique scoring criteria, along with the general strengths and weaknesses of the tools in each category, are provided. An overview of the life cycle analysis stage, functional unit, and intended users is presented in Table 2. Our primary aim in this analysis was to identify the most robust and comprehensive tools used in chemical assessment. Many of the tools presented here were developed for specific industries, products, or applications, and, as such, may not be broadly applicable for every type of chemical risk assessment.

## METHODS

Using a web-based search and input from stakeholders, a list of approximately 100 currently available chemical assessment tools was compiled. The tools could be organized into 5 categories including: life cycle assessment (e.g., GaBi), frameworks for waste reduction (e.g., P2OASys), models that predict specific physical-chemical properties (e.g., BIOWIN), or environmental fate predictions (e.g., PBT profiler), and chemical hazard or risk. As such, the chemical hazard or risk tools most commonly referenced by academia, industry groups, and regulatory agencies were selected for evaluation. Ultimately, 30 tools were evaluated, as 2 of the tools were discovered to be inactive (Table 3), and scored via a system in which tools were awarded points for fulfilling criteria developed in this analysis. Because the tools varied widely with respect to purpose and target users, they were placed into the following 4 categories so that appropriate comparisons could be made: 1) Screening and Prioritization, 2) Database Utilization, 3) Hazard Assessment, 4) Exposure and Risk Assessment, and 5) Certification and Labeling

Evaluation criteria were developed using the NSF/GCI/ANSI (NSF International/Green Chemistry Institute/American National Standards Institute) 355 Greener Chemicals and Processes Information standard and professional judgment. The NSF/GCI/ANSI 355 standard was developed by the NSF National Center for Sustainability Standards and the American Chemical Society Green Chemistry Institute through a consensus-based public process to provide a means to report the environmental aspects of a chemical and its manufacturing process over its entire life cycle (NSF International 2011).

Our evaluation criteria and scoring system are presented in Table 4. Tools were judged against nine standard criteria from which a maximum of 75 points could be awarded based on how thoroughly each criterion was incorporated into the tool. Tools were also judged against 3 supplemental criteria from which a maximum of 25 points could be awarded. As such, a maximum score of 100 points could be awarded to any one tool, with the exception of tools in the hazard assessment category. For hazard assessment tools, a maximum score of 75 points was possible, as these tools were not judged by criteria that involved exposure elements. Because the category was so large, the hazard assessment tools were divided into those that were user-driven and contained modifiable criteria and those that have fixed outputs depending on the chemical of interest. Tools with fixed outputs were further divided into those that were linked to a certification program and those that were not.

All tools were assigned either a high, medium, or low ranking, based on the numerical scores they received in the evaluation process. For tools in the hazard assessment category, the rankings were assigned as follows: high (51–75), medium (26–50), and low (0–25). For the remaining categories, the following ranking was used: high (66–100), medium (33–65), and low (0–33).

## RESULTS

The scoring criteria developed for this analysis reflect the key characteristics of a valuable chemical decision and selection tool. These characteristics included consideration for different hazard and exposure endpoints, as well as the quality of the measurements of those endpoints. A tool that had a large capacity for assessing chemicals, whether in the form of an extensive database, or in an open framework in which any chemical could be assessed was also valued over those which were more limited. Multistakeholder and consensus-based organizations that were transparent in their processes were also valued over "black-box" analyses carried out by private organizations. Our analysis also favored tools that were easy to use and that could reach a broad range of users. Grouping the tools according to their overall functionality allowed the

**Table 1**. Early chemical evaluation tools

| Category | Type | Examples | Reference |
|---|---|---|---|
| Air | Screening | Exposure and Fate Assessment Screening Tool (EFAST) | http://www.epa.gov/opptintr/exposure/pubs/efast.htm |
| | | Multi-Chamber Concentration and Exposure Model (MCCEM) | http://www.epa.gov/opptintr/exposure/pubs/mccem.htm |
| | Refined Source | Simulation Tool Kit for Indoor Air Quality and Inhalation Exposure (IAXQ) | http://www.epa.gov/nrmrl/appcd/mmd/iaq.html |
| | | Probablistic Methodology for Improving Scenario-Driven Exposure Assessment (PROMISE) | Jayjock et al. 2006 |
| | Refined Exposure | California Population Indoor Exposure Model (CPIEM) | http://www.arb.ca.gov/research/apr/past/98-327_usera.pdf |
| | | Air Pollution Exposure Model (APEX, 2.0) | http://www2.epa.gov/fera/apex-4-user-guides |
| | Point Source | Toxic Modeling System Short Term/Long Term (TOXST/LT) | EPA TOXST User's Guide EPA TOXLT User's Guide |
| | Indoor Air (Source to Air) | Multizone Airflow and Contaminant Transport Analysis Software (CONTAM) | http://www.nist.gov/el/building_environment/contam_software.cfm |
| | | IAXQ | http://www.epa.gov/nrmrl/appcd/mmd/iaq.html |
| | | MCCEM-Multi-room | www.epa.gov/opptintr/exposure/pubs/mccem.htm |
| | Microenvironment (Indirect) | CPIEM | http://www.arb.ca.gov/research/apr/past/98-327_usera.pdf |
| | | NAAQS Exposure Model (NEM)/Probalistic National Ambient Air Quality Standard Exposure Models (pNEM)/Hazardous Air Pollutant Exposure Model-MS (HAPEM-MS)/Simulation of Human Activities and Pollutant Exposure (SHAPE)/South Coast | http://nepis.epa.gov/Adobe/PDF/P10089YQ.pdf |
| | | Risk and Exposure Assessment Model (SCREAM) | http://www.epa.gov/ttn/atw/nata/sab/sabrev.html |
| | | Total Risk Integrated Methodology (TRIM)/APEX (2.0) | http://www2.epa.gov/fera/apex-4-user-guides |
| Consumer/Commercial | Screening | EFAST | http://www.epa.gov/opptintr/exposure/pubs/efast.htm |
| | | European Union System for the Evaulation of Substances (EUSES) | http://ihcp.jrc.ec.europa.eu/our_activities/public-health/risk_assessment_of_Biocides/euses/euses |
| | | Chemical Screening Tool for Exposures & Environmental Release (ChemSTEER) | http://www.epa.gov/opptintr/exposure/pubs/chemsteer.htm |
| | | ConsEXPO-3 | http://consexpo.software.informer.com/ |
| | | PROMISE | Jayjock et al. 2006 |
| | Refined | ConsEXPO-3 | http://consexpo.software.informer.com/ |
| | | PROMISE | Jayjock et al. 2006 |

**Table 1.** (*Continued*)

| Category | Type | Examples | Reference |
|---|---|---|---|
| Contaminated Sites | Screening | EFAST | http://www.epa.gov/opptintr/exposure/pubs/efast.htm |
| | | CalTOX | http://www.dtsc.ca.gov/AssessingRisk/caltox.cfm |
| | | American Petroleum Institute-Exposure and Risk Assessment Decision Support System (API-DSS) | http://www.api.org/ |
| | | SMARTRisk | http://cfpub.epa.gov/ncea/cfm/recordisplay.cfm?deid=2863 |
| | | Multimedia Environmental Pollutant Assessment System (MEPAS) | http://mepas.pnnl.gov/earth/mepasmain.stm |
| | | Multimedia Contaminant Fate, Transport, and Exposure Models (MMSOILS) | http://www2.epa.gov/exposure-assessment-models/mmsoils |
| | Refined | CalTOX | http://www.dtsc.ca.gov/AssessingRisk/caltox.cfm |
| General Diet | | Dietary Exposure Potential Model (DEPM) | http://cfpub.epa.gov/crem/knowledge_base/crem_report.cfm?deid=74901 |
| | | Dietary Exposure Evaluation Model (DEEM™) | http://www.epa.gov/scipoly/sap/meetings/2004/april/deemmanual.pdf |
| | | Communities Actively Researching Exposure Study (CARES) | http://www.eh.uc.edu/CARES/ |
| | | Stochastic Human Exposure and Dose Simulation Model for Pesticides (SHEDS-Pesticides) | http://cfpub.epa.gov/crem/knowledge_base/crem_report.cfm?deid=75824 |
| | | Lifeline™ | http://www.epa.gov/scipoly/sap/meetings/2004/april/lifelinefinaltechnicalmanual10-31.pdf |

**Table 2**. Life cycle analysis stage, functional unit, and intended users of 30 decision-support tools used to screen and prioritize chemicals

| Sector | Criteria | Criteria Explanation | Tools |
|---|---|---|---|
| Life Cycle Analysis Stage | Raw Materials Acquisition | Addresses the "cradle" stage of a product (e.g., recycled content or renewable resources) | EcoLog, EPEAT, Healthy Building Network/Pharos, Living Building Challenge |
| | Manufacture or Assembly | Accounts for chemical or product impact during manufacturing (e.g., waste created, emissions, solvents used in processing) | BOMcheck, CDAT, CleanGredients, COSHH, Cradle-to-Cradle, DfE, EcoLogo, EPEAT, Goodguide, GreenGlobes, Greenlist, GreenScreen, GreenSeal, GreenSuite, GreenWercs, Healthy Building Network/Pharos, Living Building Challenge, LCSP AA Framework, NSF ACS-GCI Standard 355 Report, RISKOFDERM, Stoffenmanager, TRA |
| | Product Distribution and Use | Evaluates effects during product distribution and use (e.g., diverse rating considerations for different products based on their variable use characteristics) | ACC Prioritization Tool, CDAT, Cradle-to-Cradle, EcoLogo, EPEAT, Goodguide, GreenGuard, GreenSeal, GreenSuite, GreenWercs, Healthy Building Network/Pharos, Healthy Building Network/Pharos, Living Building Challenge, LCSP AA Framework, SIN, TRA |
| | Product Disposal and End of Life (EOL) | Examines data from post-use phase (e.g., recyclability or reusability, chemical degradation product scores) | ACC Prioritization Tool, Cradle-to-Cradle, DfE, EcoLogo, EPEAT, Goodguide, GreenScreen, GreenSuite, GreenWercs, Healthy Building Network/Pharos, Living Building Challenge, LCSP AA Framework, RSEI, TRA |
| Functional Unit | Data | Typically associated with databases; any organized, searchable set of information | ChemHAT, CDAT, CleanGredients, CompTox, DfE, Goodguide, GreenSuite, RISKOFDERM, RSEI |
| | Chemicals | May be referred to as "ingredients;" chemical-based tools evaluate single chemicals. (e.g., benzene) | ACC Prioritization Tool, BOMcheck, ChemHAT, CDAT, CleanGredients, CompTox, COSHH, Cradle-to-Cradle, DfE, DuPont's chemical Screening Visualization Tool: Resource for Rapid Chemical Assessment, Greenlist, GreenScreen, GreenSuite, GreenWercs, Healthy Building Network/Pharos, iSUSTAIN, LCSP AA Framework, NSF ACS-GCI Standard 355 Report, RISKOFDERM, Stoffenmanager, SIN, TRA |
| | Materials | Mostly seen in building and construction tools. (e.g., wood) | BOMcheck, CleanGredients, GreenGuard, GreenSeal, GreenSuite, Healthy Building Network/Pharos, LCSP AA Framework |
| | Products | Products that contain chemical ingredients. (e.g., shampoo) | BOMcheck,COSHH, Cradle-to-Cradle, DfE, EcoLogo, EPEAT, Goodguide, GreenGuard, GreenSeal, GreenSuite, GreenWercs, Healthy Building Network/Pharos, iSUSTAIN, LCSP AA Framework, Stoffenmanager |

**Table 2.** (*Continued*)

| Sector | Criteria | Criteria Explanation | Tools |
|---|---|---|---|
| | Buildings and Infrastructure | Typically seen in certification & labeling programs where entire buildings are being evaluated against a set of criteria | GreenGlobes, GreenSeal, Healthy Building Network/ Pharos, Living Building Challenge |
| Intended User | Product Designer, Formulator, or Chemist | Person creating a new product through research and development | ACC Prioritization Tool, BOMcheck, CDAT, CleanGredients, CompTox, Cradle-to-Cradle, DfE, DuPont's chemical Screening Visualization Tool: Resource for Rapid Chemical Assessment, Goodguide, Greenlist, GreenScreen, GreenSuite, GreenWercs, iSUSTAIN, Living Building Challenge, LCSP AA Framework, NSF ACS-GCI Standard 355 Report, RISKOFDERM, TRA |
| | Suppliers | Person selling raw materials or ingredients to a manufacturer. (e.g., chemical company or textile producer) | BOMcheck, CleanGredients, COSHH, DuPont's chemical Screening Visualization Tool: Resource for Rapid Chemical Assessment, GreenSeal, GreenSuite, GreenWercs, NSF ACS-GCI Standard 355 Report, Stoffenmanager, TRA |
| | Manufacturers | Person responsible for the manufacturing plant where raw materials are turned into finished products. (e.g., a shirt factory) | BOMcheck, CleanGredients, COSHH, Cradle-to-Cradle, EcoLogo, GreenGuard, Greenlist, GreenSeal, GreenSuite, GreenWercs, Healthy Building Network/ Pharos, NSF ACS-GCI Standard 355 Report, RISKOFDERM, RSEI, Stoffenmanager, TRA |
| | Workers | Person working in manufacturing where products are made or raw materials processed. (e.g., employees of a shirt factory) | ChemHAT, COSHH, RISKOFDERM, Stoffenmanager+D23, TRA |
| | Retailers and Distributors | Entities not directly involved in the manufacturing process. (e.g., WalMart) | Goodguide, GreenGuard, GreenSeal, GreenSuite, GreenWercs |
| | Consumers | Person in the general public who purchase products from a retail store | DfE, EcoLogo, EPEAT, Goodguide, GreenGuard, GreenSeal, Healthy Building Network/Pharos, RSEI |
| | Regulators | Governmental agencies setting regulations and laws. (e.g., US EPA, ECHA, States) | ACC Prioritization Tool, CDAT, CompTox, Healthy Building Network/Pharos, LCSP AA Framework, RISKOFDERM, RSEI, TRA |
| | Specifiers | Architects, city planners, or companies who are designing buildings or infrastructure | GreenGlobes, GreenGuard, GreenSuite, Healthy Building Network/Pharos, Living Building Challenge |

**Table 3**. Category and accessibility of chemical assessment tools

| Category[a] | Tool Name | Reference | Accessibility[b] |
|---|---|---|---|
| SP, HA | ACC Prioritization Tool | http://www.americanchemistry.com/TSCA | Free |
| DB | BOMcheck | https://bomcheck.net/about | $ |
| SP, HA | ChAMP Assessment | http://www.epa.gov/champ/ | Inactive |
| DB | ChemHAT | http://www.chemhat.org/ | Free |
| SP, HA, EA | Chemical Assessment and Ranking System (CARS) | http://www.zerowaste.org/cars | Inactive |
| DB | Chemical Data Access Tool (CDAT) | http://java.epa.gov/oppt_chemical_search/ | Free |
| DB, HA | CleanGredients® | http://www.cleangredients.org/home | $$ |
| SP, DB | CompTox | http://www.epa.gov/ncct/ | Free |
| HA, EA | Control of Substances Hazardous to Health (COSHH) | http://www.hse.gov.uk/coshh/essentials/ | Free |
| HA, CL | Cradle-to-Cradle® | http://c2ccertified.org/ | $$$ |
| SP, D, HA, DF, CL | Design for the Environment | http://www.epa.gov/dfe/ | Free |
| SP, HA | DuPont's Chemical Screening Visualization Tool: Resource for Rapid Chemical Assessment | http://www.epa.gov/ncct/download_files/chemical_prioritization/Communities_of_Practice_Mario_Chen_Dupont.pdf | Free |
| CL | EcoLogo™ | http://www.ecologo.org/en/ | $-$$ |
| CL | EPEAT | http://www.epeat.net/ | Free |
| DB, HA | Goodguide | www.goodguide.com | Free |
| CL | GreenGlobes® | www.greenglobes.com | $$$$ |
| HA, CL | GreenGuard® | www.greenguard.org | $$$ |
| SP, HA | Greenlist™ | http://www.scjohnson.ca/en/scj_greenlist.aspx | $$$$ |
| SP, HA | GreenScreen ™ | http://www.cleanproduction.org/Greenscreen.php | Free |
| HA, CL | GreenSeal™ | http://www.greenseal.org/ | $$$ |
| SP, DB, HA | GreenSuite® | www.chemply.com | $$ |
| DB, HA | GreenWercs™ | http://www.thewercs.com/products-and-services/greenwercs | $$$ |
| SP, HA | Healthy Building Network/Pharos | http://www.pharosproject.net/ | $ |
| SP, HA | iSUSTAIN™ Green Chemistry Index Tool | https://www.isustain.com/ | Free |
| CL | Living Building Challenge™ | http://living-future.org/lbc | $$$$ |

**Table 3.** (*Continued*)

| Category[a] | Tool Name | Reference | Accessibility[b] |
|---|---|---|---|
| DF | Lowell Center for Sustainable Production (LCSP) AA Framework | http://www.sustainableproduction.org/downloads/FinalAltsAssess06_000.pdf | Free |
| CL | NSF ACS-GCI Standard 355 Report | http://standards.nsf.org/apps/group_public/document.php?document_id+9409 | $$ |
| HA, EA, RA | RISKOFDERM | http://www.eurofins.com/product-testing-services/services/research-development/projects-on-skin-exposure-and-protection/riskofderm-skin-exposure-and-risk-assessment/download-of-riskofderm-toolkit.aspx | Free |
| SP, DB, HA | Risk-Screening Environmental Indicators (RSEI) | http://www.epa.gov/oppt/rsei/ | Free |
| SP, HA, EA, RA | Stoffenmanager® | https://www.stoffenmanager.nl/ | Free |
| DB, HA | Substitute it Now (SIN) | http://www.chemsec.org/what-we-do/sin-list | Free |
| SP, HA, EA, RA | Targeted Risk Assessment (TRA) | http://www.ecetoc.org/tra | Free |

[a]Category: SP = screening and prioritization, HA = hazard assessment, EA = exposure assessment, DB = database, CL = certification and labeling.
[b]Accessibility: Free and publically available. $ = $1–999/yr. $$ = $1000–5000/yr. $$$ = $5000–10,000/yr. $$$$ => $10,000/yr.

same scoring criteria to be applied across the tools within each category, thereby providing a fair comparison.

### *Evaluation of all tools*

Out of a maximum score of 100, the highest score across all tools was 77. Of the 30 active tools, only 4 tools received a maximum score of 10 for assessing both hazard and exposure, while the remaining tools considered either hazard or exposure. Of the tools evaluated, 21 utilized a criteria-based assessment for each hazard endpoint, and 9 used a list-based assessment (i.e., the hazard assessment is based on the presence or absence of a chemical on a list).

Table 5 contains the results of scoring across all tools, including the average score for each criterion. Two of the criteria with the greatest room for improvement were the number of data gap provisions, as well as the review process used in developing the tools. Consideration of data gaps is important because lack of information regarding a particular hazard endpoint is not equated to a lack of potential health or environmental effect. Data gap provisions were most robust in the GreenSuite tool, which considers 5 types of data gaps, each with varying levels of impact on the final chemical hazard score. If an endpoint could not be measured for a substance because of its particular physicochemical properties, for example, the score for that chemical was not affected for having a data gap in that endpoint. On the other hand, if there was a data gap due to lack of studies on that endpoint, then the score of the chemical was penalized.

The tools with the most thorough review process were developed using established consensus standards (such as ISO or ANSI) and through peer review from a variety of disclosed, external organizations. EcoLogo, acquired by Underwriters Laboratory (UL), a third-party certification auditor of environmentally preferable products, for example, is a Type I ecolabel, as defined by the International Organization for Standardization (ISO). The program was successfully audited by the Global Ecolabelling Network (GEN) as meeting ISO 14024 standards for ecolabeling. The authors of the tool reported that stakeholders from a wide range of perspectives were selected to participate and contribute to the criteria development process. In particular, participants were sought from environmental groups, purchasers, relevant industry members and associations, consumers, and consumer groups, academia, government, and regulatory bodies, and other interested and related groups. Through a series of meetings, these stakeholders contributed to the initial draft development and subsequent draft revisions of the proposal for certification. Those tools that relied only on internal input were less favored because of the potential for bias.

### *Screening and prioritization tools*

Screening and prioritization tools aid manufacturers, regulators, and others in identifying chemicals or products that may present the highest hazard and exposure—and, thus, the highest potential risk—in a given situation. Screening and prioritization tools and frameworks are specifically created to assist with prioritization decisions. These tools generally have a high capacity for processing data and provide an output that allows for comparison across chemicals with similar functionalities. However, some of the tools evaluated were frameworks that required a more in-depth analysis that was not automated. Nine screening and prioritization tools ranked medium (33–65), and 1 tool ranked low (0–32). High-ranking screening and

**Table 4**. Summary of evaluation criteria

| Standard Criteria[a] | Available Points |
|---|---|
| Type of Assessment | |
| Hazard or exposure | 5 |
| Hazard and exposure | 10 |
| Number of Hazard Endpoints | |
| Health - acute | |
| Inhalation | +1 |
| Dermal | +1 |
| Oral | +1 |
| Health - chronic | |
| Carcinogenicity | +1 |
| Mutagenicity | +1 |
| Reproductive | +1 |
| Neurotoxicity | +1 |
| Health sub-chronic | +1 |
| Ecological Toxicity | |
| Air | +1 |
| Soil | +1 |
| Water | +1 |
| Bioaccumulation | +1 |
| Persistence | +1 |
| Flammability | +1 |
| Reactivity | +1 |
| Criteria or List Based Assessment | |
| List based | 5 |
| Criteria based | 10 |
| Data Gap Provisions | |
| One type of gap provision | 5 |
| More than one type of gap provision | 10 |
| Number of Chemicals Available for Assessment | |
| 1–99 | 1 |
| 100–999 | 2 |
| 1000–3999 | 3 |
| 4000–4999 | 4 |
| >5000 | 5 |
| Unlimited | 10 |
| Review Process | |
| Multistakeholder | +1 |
| Consensus-based | +1 |
| External peer review | +1 |
| ANSI or ISO standard basis | +2 |
| Transparency | |
| Publicly available methodology document | +2.5 |
| Disclosure of stakeholders and peer-reviewers | +2.5 |
| Ease of Use | |
| Easy input process | +2.5 |
| Easy to understand output | +2.5 |
| Accessibility | |
| Free and publicly available | 5 |
| $1–999/yr | 3 |
| $1000–5000/yr | 2 |
| $5000–10,000/yr | 1 |
| >$10,000/yr | 0 |

[a]Supplemental criteria included additional points for inclusion of additional hazard endpoints (up to 5 more points), number of exposure parameters included (up to 10 more points), and robustness of the exposure parameters (up to 10 more points).

prioritization tools (with a score of 66–100) are listed as follows, in alphabetical order:

- ACC Prioritization Tool
- GreenSuite
- Lowell Center for Sustainable Production (LCSP) AA Framework (TURI Five Chemicals Study)
- Stoffenmanager
- European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC) Targeted Risk Assessment

Ideally, tools with screening and prioritization capabilities take into account both hazard and exposure and identify chemicals or products of concern based on increased toxicity associated with a relevant route of exposure. Some of the tools had the capability to screen chemicals against a threshold, while others organized a group of chemicals into a rank order. GreenScreen is an example of a screening tool that allows users to determine a benchmark score for a chemical based on thresholds for various hazard endpoints. The resulting benchmark score reflects chemicals of high concern and potentially safer alternatives. Prioritization tools, such as Stoffenmanager, aggregate the chemical hazard information of a substance or product and combine these results with an exposure assessment to calculate a risk score followed by control measure recommendations.

Effective prioritization tools such as Stoffenmanager and the ACC Prioritization tool combine hazard and exposure ratings to yield tiers of chemicals or products that warrant further evaluation. Prioritization tools do not produce conclusions as to which chemicals present a risk to human health or environment; they can, however, present relative rankings for chemicals when compared within a particular tool. GreenSuite, for example, relies on user-modifiable

**Table 5**. Criteria scoring results for 30 decision-support tools used to screen and prioritize chemicals

| | Criteria | Points Possible | Mean | Median | Standard Deviation | Minimum/ Mean/ Maximum[a] |
|---|---|---|---|---|---|---|
| | Hazard and/or exposure | 10 | 5.3 | 5 | 1.8 | |
| | # of hazard endpoints | 15 | 7.3 | 6.5 | 4.8 | |
| | Criteria or list-based | 10 | 8.2 | 10 | 3.1 | |
| Standard Scoring | Data gap provisions | 10 | 3.3 | 2.5 | 3.8 | 20/42/60 |
| | # of chemicals for assessment | 10 | 6.3 | 5 | 3.8 | |
| | Review process | 5 | 2.7 | 3 | 1.4 | |
| | Transparency | 5 | 3.7 | 5 | 1.7 | |
| | Ease of use | 5 | 3.1 | 2.5 | 1.8 | |
| | Accessibility | 5 | 3.5 | 5 | 1.9 | |
| | Additional hazard endpoints | 5 | 2.1 | 2 | 2.1 | |
| Supplemental Scoring | # of exposure parameters | 10 | 3.4 | 5 | 3.5 | 0/8.2/25 |
| | Robustness of exposure parameters | 10 | 2.8 | 0.5 | 3.8 | |

Scoring based on the evaluation of 30 tools.
[a]Combined score across all criteria for the 30 tools evaluated.

criteria to determine the "green" score for a chemical or mixture. Although the tool is primarily hazard-based, it is capable of providing a 0–100 score very quickly, thus allowing for numerous chemicals to be compared against one another.

The Lowell Center for Sustainable Production has published extensive guidance on the process of Alternatives Analysis (AA). This guidance is general in nature, so it is applicable to many situations. To assist in scoring the AA guidance put forth by LCSP, we used the Five Chemicals Study, published by an LCSP affiliate, to understand how the LCSP's alternatives assessment framework is implemented. The initial step in the Five Chemicals Study was to select priority categories of use for each chemical and to evaluate potential alternatives for the chemical in that particular use. Once the alternatives were identified and an initial screen was performed by the researchers, the remaining alternatives were prioritized for further evaluation based on feasibility, health and environmental effects, and economic considerations.

### *Database tools*

Tools evaluated within the database category included tools that are standalone databases, as well as tools with a database component. Many of these are web-based tools that allow for querying a product or chemical. Among the tools analyzed, some utilized databases of regulatory lists, material safety data sheets (MSDS), and chemical toxicity information. The key qualities of database tools include frequent and consistent updates, a large volume of data, and an easy-to-navigate user interface. Seven database tools ranked medium (33–65), and 2 ranked low (0–32). High-ranking database tools (with a score of 66–100) are listed as follows, in alphabetical order:

- GreenSuite
- RISKOFDERM

We found GreenSuite and RISKOFDERM to be two very different, yet powerful, tools in this category. GreenSuite is a web-based tool that pulls from an extensive database of health and safety information for 275 000 chemicals, more than 1 500 000 product MSDS, and over 800 regulatory reference lists. According to the tool developer, updates are made annually to the database and also as needed throughout the year. RISKOFDERM was developed as a predictive model for estimating dermal exposure, and as a practical dermal exposure risk assessment and management toolkit for use in the workplace. It has also resulted in a large volume of dermal exposure data that has been compiled in multiple databases (van Hemmen et al. 2003).

### *Hazard assessment tools*

Hazard assessment tools are defined as those that generate an output related to the potential health hazard of a chemical or product. The majority of the tools evaluated were hazard assessment tools. Fourteen hazard assessment tools ranked medium (26–50); one ranked low (0–25). High-ranking hazard assessment tools (with a score of 51–75) are listed as follows, in alphabetical order:

User-modifiable criteria hazard assessment tools:

- GreenSuite
- GreenWercs

Fixed-criteria hazard assessment tools (not linked to certification):

- Design for the Environment
- GreenScreen
- iSUSTAIN

GreenSuite scored highly in the category of hazard assessment with user-modifiable criteria. In terms of chemical evaluation, the tool provides a "green score" based on 44 ecological, health, and safety criteria. Scoring defaults to a built-in weighting system that can be overridden with the user's own preferred weighting. The weight of the health endpoints, for example, can be increased or decreased relative to the ecological and safety endpoints. Furthermore, weights for each of the 44 criteria can be customized. When a chemical is evaluated, all 44 endpoints are taken into account to calculate the overall green score. Also available is the degree of certainty, which is a reflection of the number and types of data gaps for that chemical. Data gaps are scored differently (also customizable), depending on the nature of the missing information.

GreenWERCS, an example of a hazard assessment with user-modifiable criteria, is a program that allows users to understand the overall health and environmental impacts of their product through a scoring system. Additionally, users can view which ingredients are driving the score based on the percent composition in the product. The scoring system is based on user-defined criteria that weights different hazard endpoints. GreenWERCS also includes a default scoring system through inclusion of the GreenScreen List Translator, which is the portion of the GreenScreen method that is drawn from 850 hazard lists and 36 authoritative (as defined by Clean Production Action) sources. The incorporation of GreenScreen List Translator functionality enables the user to quickly screen against the GreenScreen List criteria and to perform the first phase of the full GreenScreen methodology. The GreenWERCs tool is also customizable, allowing the user to specify all or some of the embedded hazard lists or authoritative sources. In general, little technical expertise is required to run an analysis, and the user interface is relatively simple.

USEPA's Design for the Environment (DfE) is a comprehensive program that consists of product labeling and ingredient evaluation. At the center of the DfE program, however, is the Alternatives Assessment Criteria for Hazard Evaluation, which is a series of 'high', 'medium', or 'low' designations for numerous human health and environmental toxicity and fate endpoints. Using these fixed criteria, numerous human health and environmental toxicity and fate endpoints can be designated as being of 'high', 'medium', or 'low' concern. The criteria for these designations are based on international recognized standards, including the United Nation's Globally Harmonized System (GHS) for the Classification and Labelling of Chemicals and EU REACH, as well as USEPA programs, such as the USEPA Endocrine Disruptor Screening Program, and the USEPA Office of Pollution Prevention & Toxics criteria for high production volume (HPV) chemical categorization.

GreenScreen's fixed criteria hazard assessment tool builds on the DfE program, and serves as a decision-making aid by taking data on human health and ecological endpoints and prioritizing those characteristics. Users score each chemical and its degradation products with a 'very low' to 'very high' mark in categories related to chronic and acute health effects, as well as environmental and physical characteristics. Each entry on the hazard rating matrix corresponds to a specific, quantitative, or qualitative guideline for what qualifies as a very low, low, medium, high, or very high hazard. These scores are derived from various authoritative and screening sources. Once the hazard matrix has been completed, the user can identify an overall benchmark score for the chemical. Many considerations must be made when assigning a benchmark, such as the hazard properties of the degradation products and the number of data gaps in the table. Benchmark 1 chemicals are considered high concern, and should be avoided; Benchmark 2 chemicals are acceptable for use, but alternatives are still recommended; Benchmark 3 chemicals are preferable to Benchmark 1 and 2 chemicals but still leave room for improvement; and Benchmark 4 chemicals are preferred and considered safe.

The iSUSTAIN Green Chemistry Index is an internet-based sustainability scoring tool that was designed to rapidly evaluate products or processes using readily available information. iSUSTAIN generates separate scores for each of the following 12 metrics based on the Principles of Green Chemistry, and requires the user to enter information pertaining to the Bill of Materials (BOM) in, the BOM out, and the process steps. Each of the 12 metrics has a prescribed scoring system (comprised of different subscores) that is relevant to the particular sustainability principle. For example, scoring for the Safe Raw Material, Safe Product, and Safe Solvent metrics is based on available safety, health, and environmental information; currently, European risk phrases are used as the primary information source. The Safer Chemical category is comprised of subscores for both aquatic and human toxicity, and pre-assigned scoring or new scores can be selected. Additionally, for the Safe Product category, when European risk phrases are not available, environmental exposure data are derived using models (e.g., USEPA ECOSAR), and literature searches are conducted for acute and chronic effects. Resultant scores for each metric can range from 0 to 100 (100 is best), and the end result is plotted on a radial graph for that particular material or process, and can be compared to others.

The Pharos project is a certification and labeling program with a fixed criteria hazard assessment component. It consists of two libraries: the Building Product Library and the Chemical and Material Library. The Building Product Library is divided into 13 product categories consisting of adhesives, ceilings, composite wood, countertops, decorative laminates, floor sealants and coatings, flooring, high performance coatings, interior paint, roofing membranes, thermal insulation, wall protection, and wallboard. Within the Building Product Library, the products are scored based on hazards relating to volatile organic compounds (VOCs), toxic content (ToxCon), manufacturing toxics (MfrTox), renewable materials (RnMtrl), renewable energy (RnEnrg), and, within the roofing products section only, reflectance (Reflct). Information is provided by manufacturer participation and disclosure, as well as from research performed by Pharos. Once reviewed, the Pharos team assigns the chemical color based on the corresponding GreenScreen benchmark. Colors are assigned based on high to low hazard. Within the Chemical and Materials Library, Pharos screens those materials using the GreenScreen benchmarking system to identify potential health hazards for those exposed to the material. Persistent bioaccumulative toxicants (PBTs) receive the highest priority for elimination, followed by priority health effects: cancer, genetic mutation, reproductive or developmental harm, and endocrine disruption. Additionally, the Pharos team identifies the potential life cycle health hazards, and screens these chemicals to identify potential health hazards to the workers and local communities near where the raw materials are mined or grown and then manufactured into products. The Pharos team then assigns a chemical color based on the outcomes. Once again, colors are assigned based on high to low hazard, or black to green.

### *Exposure and risk assessment tools*

Exposure and risk assessment tools are capable of quantifying the estimated exposure of an individual based on chemical or product-specific information. These tools are fully capable of predicting exposure, and can be considered risk assessment tools in the traditional sense. They have the capacity to predict risk based on a combination of hazard and exposure data, whether modeled or collected. The majority of the exposure and risk assessment tools we evaluated were REACH exposure assessment tools. Under the REACH program, chemicals are first separated into tonnage bands as a proxy for exposure, such that chemicals that have the highest total manufactured or imported mass can be prioritized. For all substances produced at ten tons or more per year, an individual risk assessment for the chemical must be carried out. These assessments, known as chemical safety assessments, are composed of a human health hazard assessment, environmental hazard assessment, persistent, bioaccumulative, and toxic (PBT) assessment, exposure assessment, and risk characterization (Sahmel 2012). Registered substances that meet the criteria to be considered hazardous are also required to have an exposure assessment and risk characterization of varying complexities, depending on the tonnage band of that substance. Tier 0 assessments are the most basic, and rely on conservative default assumptions. Tier 1 assessments, which include all of the exposure and risk assessment tools in this analysis, consider chemical hazard, exposure scenarios, and use information in order to evaluate risk. Lastly, Tier 2 assessments are detailed risk assessments reserved for chemicals that have demonstrated potential concerns (Sahmel 2012). One exposure assessment tool ranked medium (33–65). High-ranking exposure assessment tools (with a score of 66–100) are listed as follows, in alphabetical order:

- RISK OF DERM
- Stoffenmanager
- TRA

Overall, the quality of exposure assessments in the selected tools varied greatly. Many tools indicated that they considered exposure, but relied solely on proxy measurements, such as the percent concentration of a chemical in a product or production volume estimates. While these measures may be acceptable as an initial screen or as a way to group chemicals at a high level, they do not qualify as exposure metrics when calculating chemical risk. For that, relying on measured or modeled data specific to each relevant route of exposure is necessary. All tools in this category relied on the input of actual exposure data.

Within the exposure assessment tools category, the manner in which the tools conducted an exposure characterization spanned a wide range in terms of sophistication. For instance, one of the primary drawbacks of the COSHH tool is that it depends on control banding, and does not give an exposure or risk score. Stoffenmanager is similar to the COSHH toolkit, but has the added capability of determining a risk score and relative risk ranking score for a particular chemical use scenario. RISKOFDERM provides excellent data on dermal exposure patterns and has enabled improved dermal risk assessment and management in the manufacturing environment. One deficit we found, though, was the availability of consumer product-oriented risk assessment tools. The majority of the tools we evaluated in the exposure and risk assessment space were geared towards occupational settings, although the Targeted Risk Assessment (TRA) tool, developed by the European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC), did have a consumer product capacity.

TRA consists of 3 separate models for estimating exposure to workers, consumers, and the environment. These modules are based on exposure scenarios. TRA is a risk assessment tool that allows the user to evaluate the potential risk of a chemical in a product for a specific use. It is available for download as a comprehensive program of all 3 modules, or as just the consumer product module by itself. A risk ratio is calculated using information on a chemical's toxicity criteria (i.e., reference concentration or dose or derived no effect level) which is then compared to the potential exposure. The user must input information on the chemical properties and uses of the chemical. Default exposure values are built in, including those related to volatility, dermal contact, and oral exposure, although these can be modified. The output is a risk ratio (RR) that compares the predicted exposure to the acceptable level where a risk ratio $<1$ is considered acceptable. For human health, this ratio is calculated as: RR = Predicted Environmental Concentration / Derived No-Effect Levels (DNEL). TRA is accepted as a tier one assessment tool for inhalation and dermal exposures, and is the only consumer product tool that provides an understanding of risk from an ingredient in a product

### *Certification and labeling tools*

Certification and labeling programs included various ecolabels and the supporting certification programs. These tools provide a positive outcome for the user in the form of documentation indicating that the chemical or product complies with certain criteria. We ranked the various certifications and labeling programs based on the how they developed their standards and the robustness of their chemical hazard evaluations. Programs in this category spanned a broad range of industries, from electronics to building and construction and cleaning products, and chemical or building material health was generally just one of many components. The certification and labeling programs generally did not receive high scores because they lacked robust hazard and exposure criteria, and primarily focused on evaluating energy requirements, water usage, and end-of-life management of products, which, while important for the overall evaluation of a product's life cycle, were not considered in our scoring scheme. One exception was the DfE Safer Product Labeling, which had the highest ranking (64).

In addition to the aforementioned hazard evaluation, DfE also recognizes safer products through a labeling program. Safer Product Labeling is one of the DfE's current partnerships. Through this program, DfE evaluates products, and awards its label to those that meet its criteria. Currently, most products achieving DfE certification are cleaners. DfE labels a variety of chemical-based products, including all-purpose cleaners, laundry detergents, and carpet and floor care products. At present, there are more than 2 800 products that carry this label. A participating company must be willing to submit all of the product ingredients to DfE and a qualified third party profiler, who then compiles hazard information on each chemical, including the detailed structure, physical-chemical properties, human health and environmental toxicology, and regulatory and administrative status.

## DISCUSSION

The importance of robust hazard and exposure assessments cannot be understated. Our analysis favored hazard evaluations that were based on endpoint-specific criteria over list-based assessments. Authoritative lists were viewed as lagging indicators, in that the evaluation of the chemical has already been carried out, and the chemical has likely already been marked for deselection. Tools that relied solely on red or black lists were considered to be overly exclusive, as they did not consider risk based on exposure potential or use considerations before characterizing the chemical as undesirable. What may be more valuable is a tiered approach that utilizes an authoritative or regulatory list as an initial screen when assessing large groups of chemicals. As another approach, tools such as DfE and GreenScreen rely on a combination of criteria and list-based assessment, referring to a hierarchy of authoritative lists for information on some hazard endpoints, while establishing toxicity thresholds for others.

Although the majority of the top ranked hazard assessment tools included 7 or more toxicity endpoints, several additional endpoints, including endocrine disruption, phototoxicity, and metabolite toxicity are emerging as hazard considerations that the tools will need to incorporate. However, little available information or a lack of agreement in terms of assessing the severity or importance of these effects is often a problem. To date, the most significant effort has been on the assessment of endocrine disruption activity, where screening programs have been initiated in the US and are pending development in Europe. The Organization for Economic Cooperation and Development (OECD) has published a series of test methods in conjunction with the USEPA to address the multiple modes of actions upon which a chemical may exert endocrine disruption (Gelbke et al. 2004). Final criteria for classifying a chemical as an endocrine disrupter are still in flux, although GreenScreen has proposed a scoring scheme for this endpoint.

Given the plethora of tools available, finding the most appropriate one for use may be difficult, and often the name or description of the tool is not helpful. During the tools assessment, occasionally a discrepancy between the original intended use of the tool and its current use in the marketplace occurred. Generally the tools that lacked automation, such as DfE and GreenScreen, require a much more sophisticated user, with specific skill sets in toxicology and exposure assessment, than do those in which the hazard and exposure information could be generated through a computer program. If companies lack trained technical staff to perform the chemical assessments, they should consider those tools that automate the hazard assessment, but should recognize that the screening may only be based on others' lists, and that the exposure scenarios may be based on default assumptions that do not apply to every specific chemical or product.

Given that the maximum score across all tools was 77 out of 100, there is clearly room for improvement, even among the highest scoring tools. Our general recommendations for improving the tools include: combining existing hazard and exposure tools to provide an ability to screen and prioritize based on risk; incorporating data gap considerations; increasing transparency of the tools, methods, assumptions, and external peer review; providing options for emerging endpoints (endocrine disruption, phototoxicity, metabolites, etc.), and automating manual hazard endpoint look ups to make the tools more accessible and increase capacity.

In the US, there are currently hundreds of policies both enacted and pending regarding regulation of chemicals in consumer products. Recent examples of chemical hazards and risk regulation policies include initiatives enacted in California, Maine, Minnesota, Oregon, Washington, and Wisconsin, among others. In fact, the number of policies involving chemical regulation has grown tremendously in the last decade, with almost 100 policies pertaining to Alternatives Assessments adopted across the 50 states from 2005 to 2010, compared to none in the prior 5 years (IC2 2011). Further, several of the state policies either endorse or require using specific chemical assessment tools to identify or assess hazards (Maine Department of Environmental Protection 2010; SoW 2013). Additionally, the retail sector (including companies such as Target and WalMart) has increased demands for chemical assessment tools, and some retailers have endorsed or require use of specific chemical assessment tools from their suppliers. The results of these tools-based analyses directly translate into the availability of the products on shelves and, by extension, the ultimate viability of those products in the marketplace.

Evidence suggests that the tools we evaluated—and others like them—will continue to play a role in chemical and product evaluations at the regulatory level and throughout various supply chains. As such, understanding the relative strengths and weaknesses of each becomes increasingly valuable. The analysis herein provides an objective characterization of popular chemical assessment tools and serves as a reference for those using them or specifying their use. A number of tools scored well in our evaluation, but all revealed areas in which improvements could be made. In particular, many of the tools lacked the capability to evaluate risk based on exposure. Too many tools, in our opinion, were solely hazard-based or dependent on restricted chemicals lists.

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