**SUPPLEMENTARY INFORMATION**

**Advancing green chemistry performance assessment:** **The Estée Lauder Companies’ continuing journey towards meaningful transparency**

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# 1. Scoring rubrics for each enhanced Green Score metric

**Table S1.** Scoring rubrics for each enhanced Green Score metric. Rubrics are listed in order of metric description within the Methodology section. GHG, greenhouse gas; LCA, life cycle assessment; LCI, life cycle inventory, CO2e, carbon dioxide equivalent; ELC, the Estée Lauder Companies. Final ingredient and formula scores are transformed to a 0-100 scale for ease of formulator understanding.

|  |  |  |
| --- | --- | --- |
| **Metric Description/Source** | **Score** | **Score Assignment Rubric** |
| **Waste:** Assesses for the volume of generated chemical waste and degree of process hazard across the ingredient’s full manufacturing supply chain. Empirical supplier E-factor and process hazard data was prioritized. If not available, estimated E-factor and process hazard proxies derived from a literature-based model were assigned, per component identity, source, and manufacturing process. The E-factor scaling equation was selected to best fit the data distribution and differentiate between the most commonly observed values. | **1** | E-factor > 100 |
| **5-2\*log(e-factor)** | E-factor ≥ 1 |
| **5** | E-factor < 1 |
| **-0.5 point** | Processing entails high hazard |
| **+ 0 points** | Processing entails intermediate hazard / lack of data |
| **+0.5 point** | Processing entails low hazard |
| **Degradation:** Assesses the ingredient’s propensity to break down in aquatic environmental conditions. Refer to Table 1 for criteria and definitions. | **1** | Persistent |
| **2** | Uncertain (potentially) persistent |
| **3** | Non persistent OR feedstock source is wholly inorganic |
| **4** | Inherently biodegradable |
| **5** | Readily biodegradable |
| **GHG emissions:** Assesses for ingredient’s cradle-to-gate GHG impact. Empirical, supplier LCA derived data was prioritized. If not available, estimated emissions factor proxies obtained from relevant LCI databases were assigned, per component identity, source, and manufacturing process. All emissions factors utilized units of kg CO2e/kg material produced. The metric scaling equation was updated to best fit the new data distribution and differentiate between the most commonly observed emissions factors. | **1** | Supplier or proxy carbon emissions factor > 15.5 |
| **6.5-2\*x0.37** | 0.55 ≤ supplier or proxy carbon emissions factor ≤ 15.5 |
| **5** | Supplier or proxy carbon emissions factor < 0.55 |
| **Feedstock sourcing:** Assesses for ingredient renewability, traceability to country of origin (COO), and possession of a third-party sustainability certification. Natural origin index (NOI) is calculated internally per supplier data according to ISO 16128 guidance, with all other metric data obtained from ELC suppliers. | **1** | Ingredient NOI is <50% |
| **4\*((x/100))-1** | 50% ≤ Ingredient NOI < 100% |
| **3** | Ingredient NOI is 100% |
| **+1 point** | All components have known COOs |
| **+1 point** | Ingredient has third-party sustainability certification |

# 2. Waste metric E-factor calculation parameters

**Table S2.** E-Factor calculation parameters, as stipulated by ELC for assessment of ingredient waste impacts.

|  |  |
| --- | --- |
| **In-Scope Waste Factors** | **Out-of-Scope Waste Factors** |
| -Chemical waste across the full manufacturing supply chain (*i.e.*, byproducts, auxiliaries, solvents, *etc*.)  - Initial feedstock processing (*e.g.*, non-directly backfilled mining waste) | - Residual biomass, including that resulting from biotechnological processes  - Energy use and electricity production  - Purification  - Water use |

# 3. Certainty score assignment

As previously reported, each Green Score metric features a corresponding certainty score, which provides insight into the quality and robustness of underlying data.1 Certainty scores serve as a forward-facing indicator for formulation teams but are not influential to the actual raw material Green Score. V.2.0 certainty scores follow the same general framework as Green Score v.1.0, with select adjustments to best reward the use of newly incorporated, highly robust data (i.e., empirical test results and validated supplier data) and consider non-empirical, less robust data more conservatively.

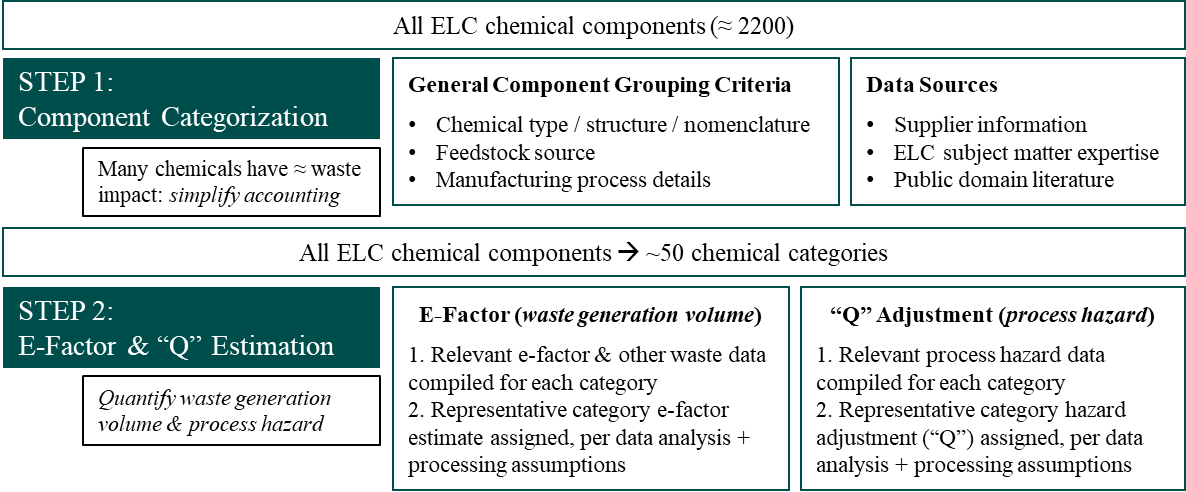
**Table S3.** Certainty score assignment rubrics for each enhanced Green Score metric, listed in order of metric description within the Methodology section. Certainty score assignment was based on the quality and availability of underlying component data. EQ, environmental quotient; DSL, Domestic Substance List; QSAR, quantitative structure–activity relationship; OECD, Organization for Economic Co-operation and Development; RIFM, Research Institute for Fragrance Materials; GHG, greenhouse gas; LCI, life cycle inventory; LCA, life cycle assessment; ISO, International Standards Organization.

|  |  |  |
| --- | --- | --- |
| **Metric** | **Certainty Score** | **Description** |
| Waste | 2 | EQ-factor solely from modelled data |
| 3 | E-factor from supplier data; “Q” from modelled data (or vice versa) |
| 5 | EQ-factor solely from validated empirical supplier data |
| Degradation | 1 | Default score (no data available) |
| 3 | Component score from Canada DSL or QSAR modelling (weight of evidence approach) |
| 4 | Component score derived from properly justified read across or scientific literature |
| 5 | Component score derived from OECD test results (per supplier, RIFM, etc.) or the Detergent Ingredients Database list |
| GHG Emissions | 2 | Score derived from default mapping to LCI database entry or scientific literature |
| 4 | Score derived from direct mapping to LCI database entry or scientific literature |
| 5 | Score derived from validated supplier LCA |
| Feedstock Sourcing | 3 | Score derived from supplier provided binary data |
| 5 | Score derived from ISO Natural Origin value |

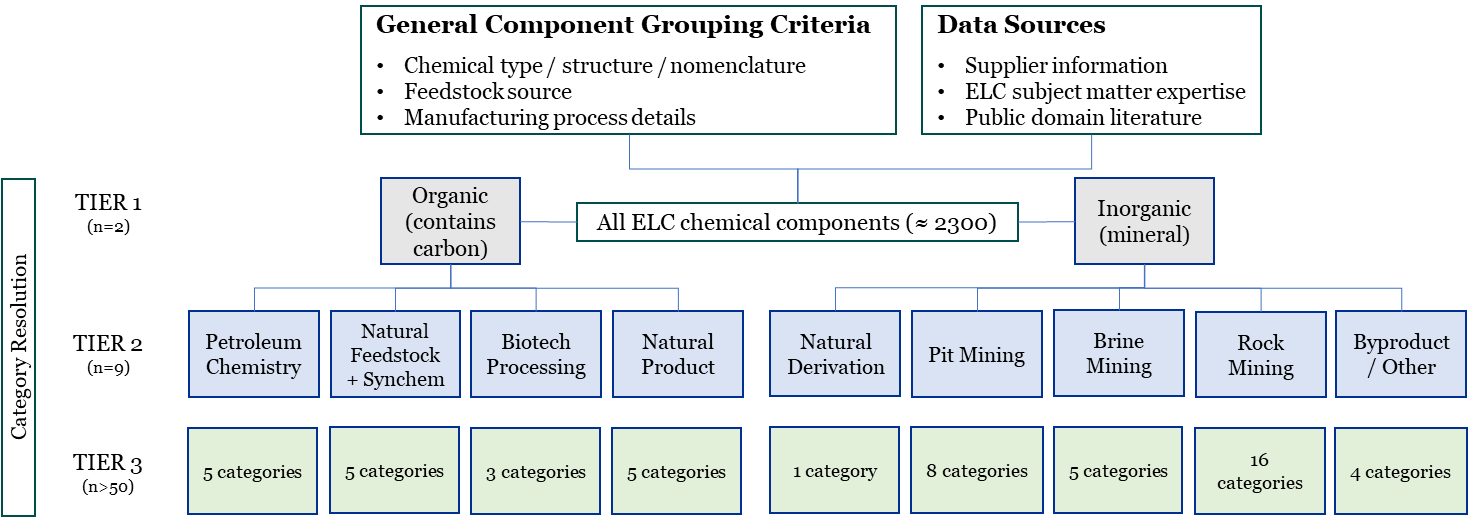
# 4. Waste model development

The waste model estimates ingredient EQ-factors through a streamlined accounting approach predicated on life cycle inventory, but solely focused on waste volume (E-factor) and process hazard impact.2-4 Data was first estimated at the component level before being aggregated to the ingredient level, in alignment with the other Green Score endpoints. Representative E-factor and “Q” values were assigned to each component category as per ‘nearest neighbor’ literature results. Development of the model is visualized in Figure S1, with Step 1 grouping ELC chemical components into approximately 50 categories, based on similarities in respective chemical identity, feedstock, and manufacturing process. While the cosmetics industry uses chemical components from varying sources (i.e., mineral, biological, petroleum), this categorization stemmed from the assumption that there is sufficient similarity in manufacturing processes amongst certain discrete groups of components that their waste impact can be considered equivalent.5-8 Categorization was performed according to internal ELC expert judgement, with further details on the underlying criteria, rationale, and assimilated data sources provided in Figures S2, S3 and S4.

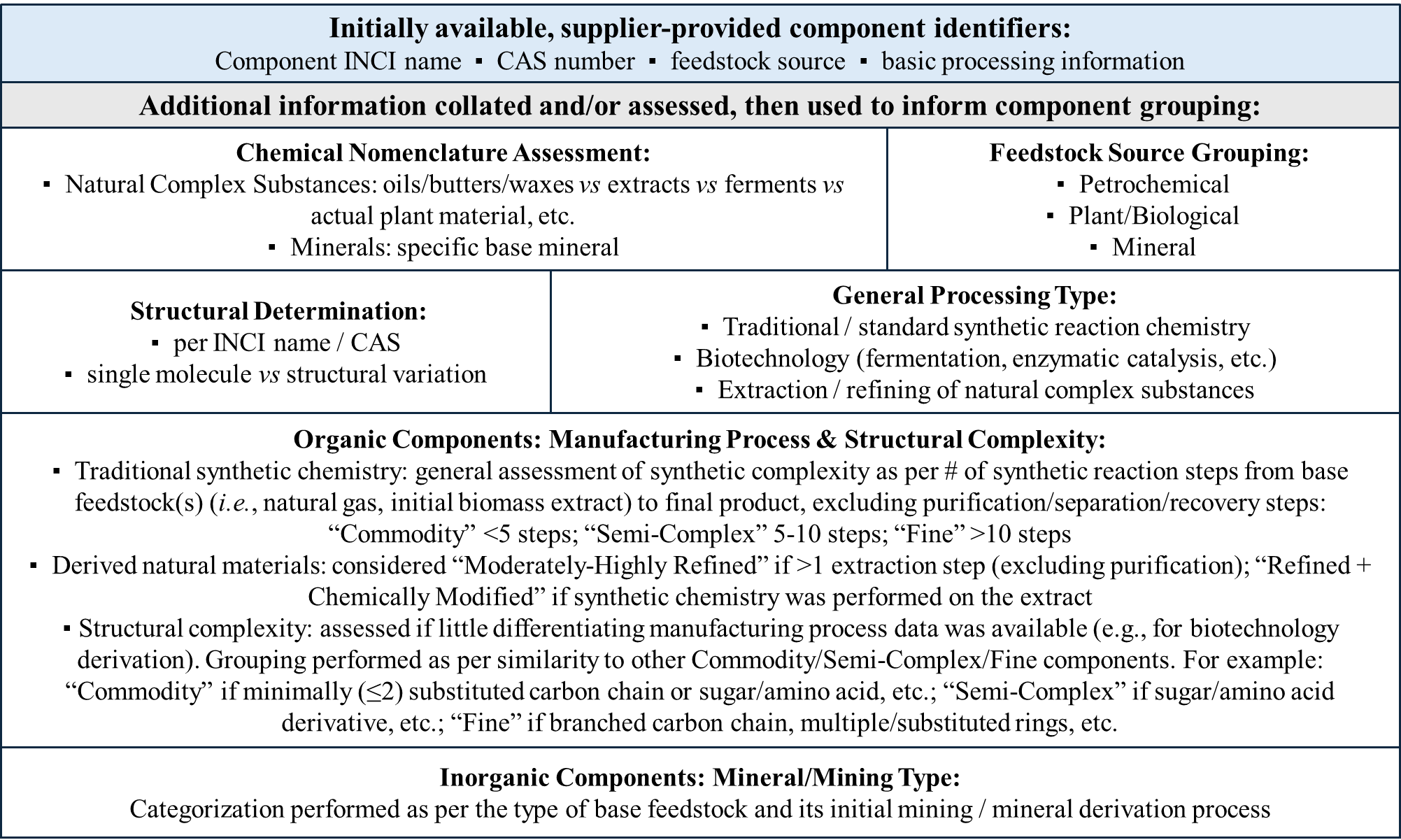
Step 2 of the waste model development (Figure S1) entailed assigning a single representative E-factor estimate and hazard adjustment (“Q”) to each chemical category. Estimates were derived from an extensive literature and patent search of chemicals with similar structures and manufacturing processes to the types of chemistries used in cosmetic formulas. Beyond reported E-factors and process conditions, additional data relevant to waste generation (*e.g.*, mining byproducts) was also collated. Special emphasis was placed on investigating the waste generation impact of feedstock processing to enable consideration of the full manufacturing supply chain. Category value estimation was then performed based on assessment of the most relevant datapoints for each category. Specifically, this entailed considering the relevance of experimental calculation parameters and process conditions (*e.g.*, degree of process optimization), along with the extent of process coverage across the full supply chain. Figure S5 provides a stepwise overview of the E-factor and “Q” value assignment process, and Figure S6 contextualizes the process through a worked example of value derivation for a representative chemical, butylene glycol, with two different manufacturing routes. Tables S4-6 provide further details into the base data set and specifics of E-factor and “Q” value assignment, such as special considerations for inorganic chemistries.



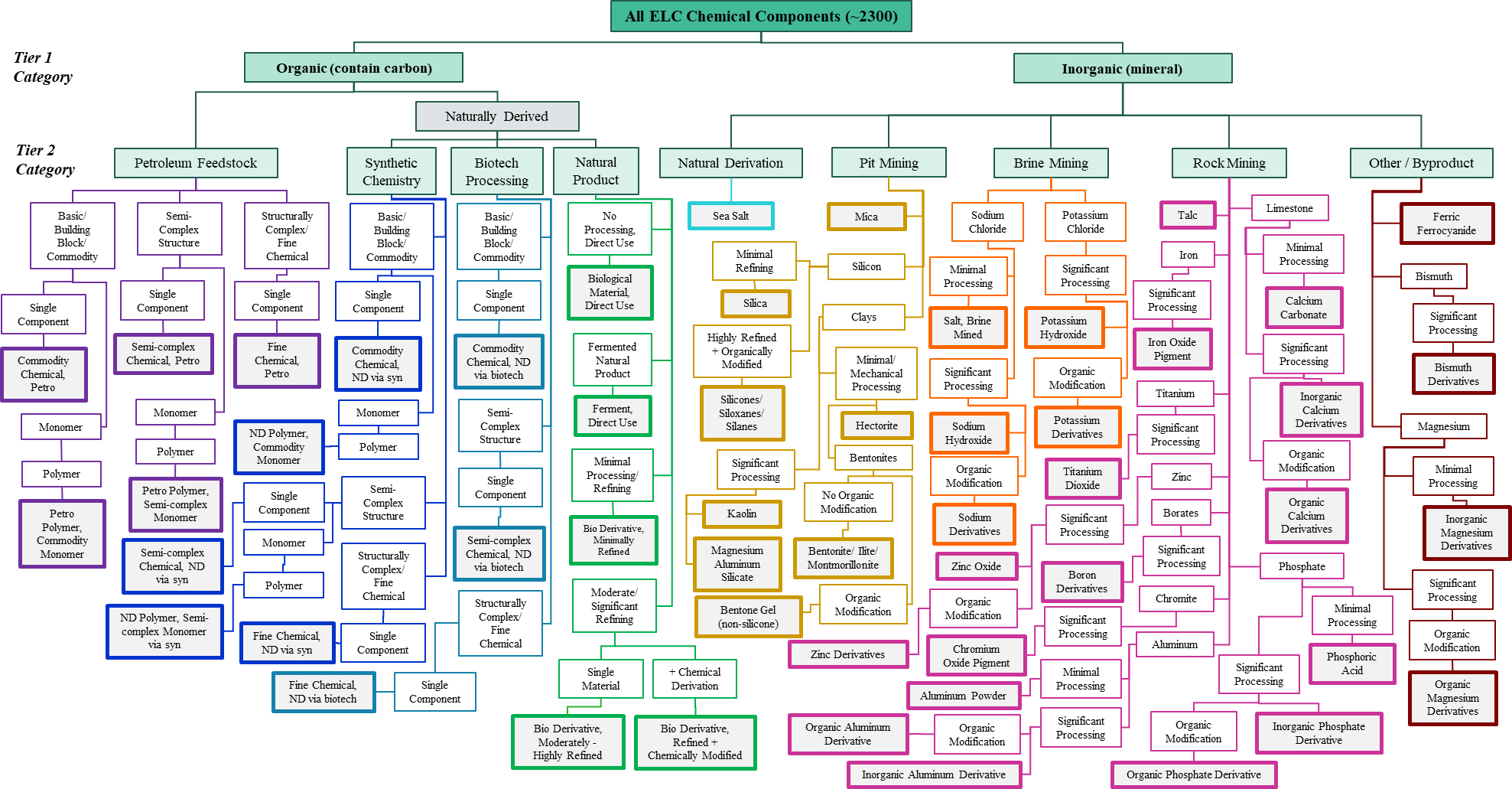
**Figure S1.** General schematic overview of the EQ-factor model development.



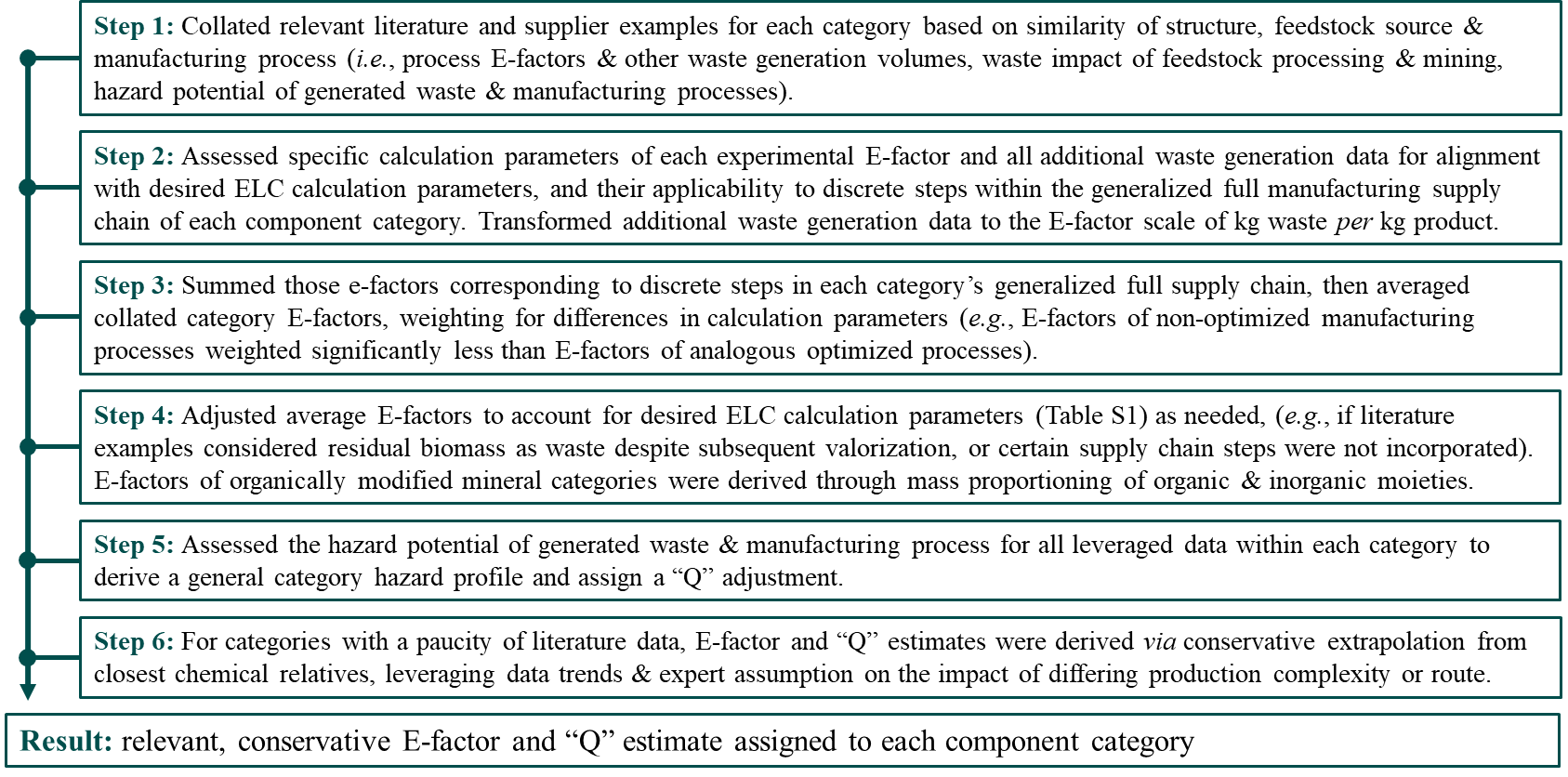
**Figure S2.** Overview of chemical component categorization process. Categorization ensured that similar structural analogues, with similar feedstocks and manufacturing processes, were assigned the same representative E-factor estimate. This approach was generally analogous to that previously adopted for the GHG modelled emissions endpoint categorization. Organic and inorganic components were first differentiated to ensure that the unique sourcing (i.e., mining or mineral derivation) and manufacturing processes of inorganics were sufficiently addressed. Figure S3 provides an overview of the data sources and considerations used to derive each component’s Tier 1, 2 & 3 groupings, with all specific Tier 1, 2 & 3 category options visualized in Figure S4. Synchem, synthetic chemistry.



**Figure S3.** Specific data sources and considerations underlying the grouping of chemical components into representative Tier 1, 2 & 3 categories, as performed utilizing ELC expert judgement. For naturally derived components manufactured via traditional synthetic chemistry or biotechnology, initial biomass processing was excluded to not overly penalize them versus petroleum derived materials, as crude petroleum/natural gas is also refined and/or cracked prior to chemical synthesis.



**Figure S4.** Dendrogram of the Tier 1, 2 & 3 component categories (Figure S2). Boxes with bolded outline represent the Tier 3 component categories. Boxes with non-bolded outline represent generalized upstream manufacturing process steps and relevant process attributes, and are delineated to aid understanding. Bio, biological (including botanicals); biotech; biotechnological processing; ND, naturally derived; petro, petroleum; syn, synthetic chemistry.



**Figure S5.** Overview of the derivation process for category E-factor and “Q” estimates based on literature data and manufacturing process assumptions. Special considerations were taken for the derivation of E-factor and “Q” estimates for inorganics, to ensure they were not overly penalized versus organics due to differences in feedstock obtention and processing. For instance, mining byproducts that could be directly returned to the mine after closure (*e.g.*, non-ore containing rocks or soil) were not considered waste, whereas byproducts that could not be directly returned to the mine after closure, such as hazardous tailings requiring sequestration or treatment, were considered waste. All byproducts of downstream ore processing were also considered waste unless explicitly stated as recycled or valorized.

A screenshot of a computer

Description automatically generated

**Figure S6.** Worked example of modelled category E-factor and “Q” derivation utilizing butylene glycol shown with two contrasting derivation routes.

# 5. Waste model underlying data and value estimates

**Table S4.** EQ-factor model categories, values, underlying literature and supplier data, and commentary on expert judgement based value assignments for organics categories.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Component Category** | **E-Factor** | **“Q” Adjustment** | **Underlying Source Data** | **Commentary** |
| Commodity, petro | 2 | Penalty | <1-5 (standard literature values)9  0.1-1.5 (7 literature calculations; majority <1; all optimized processes; starting materials production excluded)10-16 | Estimate including starting materials |
| Commodity, renewable via chemical synthesis | 3 |  | 0.02-3.4 (14 literature calculations; optimized & non-optimized process; starting materials production generally excluded; calculation parameters vary)10, 14, 15, 17-19 | Estimate including starting materials and assuming valorization / recycling of waste biomass |
| Commodity, renewable via fermentation / biotechnology | 4 | Bonus | 1.19-31.4 (7 literature calculations; optimized & non-optimized process; starting materials production generally excluded; some include water; calculation parameters vary)11-14, 16, 20 | Estimate including starting materials and assuming valorization / recycling of waste biomass |
| Semi-complex, petro | 7 | Penalty | 1.28 (1 literature calculation; modelled optimized process; starting materials production excluded)21 | Middle ground of commodity and fine; reflects petrochemistry efficiency with synthesizing simpler molecules |
| Semi-complex, renewable via chemical synthesis | 8 |  | 0.08-1.77 (3 literature calculations; optimized processes; starting materials production excluded)21-23 | Assume similar to semi-complex, petro |
| Semi-complex, renewable via fermentation / biotechnology | 7 | Bonus | No specific examples – extrapolated from closest chemical analogues | Middle ground of commodity and fine; reflects directionality of assessed data and other categories |
| Fine, petro | 15 | Penalty | 5-50 (standard literature values)9  8-13.8 (2 literature calculations; optimized processes; starting materials production excluded)24-26 | Cosmetic chemistries are generally less structurally complex than pharmaceuticals; estimate including starting materials |
| Fine, renewable via chemical synthesis | 16 |  | 1.2-161 (18 literature calculations; optimized & non-optimized process; calculation parameters vary; some include water; most well under 16; starting materials production excluded)27, 28 | Estimate including starting materials and assuming valorization / recycling of waste biomass |
| Fine, renewable via fermentation / biotechnology | 10 | Bonus | 0.06-82.5 (10 literature calculations; optimized & non-optimized process; most include water or purification & consider residual biomass as waste though it could be valorized; starting materials production generally excluded)29-33 | Estimate including starting materials and assuming valorization / recycling of waste biomass. While estimate of 10 is conservative, it does not account for energy / water purification requirements. |
| Polymer, commodity monomer, petro | 3 | Penalty | ~0 to <1 (9 literature calculations of only polymerization process; starting materials production excluded)34 | Estimate including starting materials; polymerization is generally low in waste generation |
| Polymer, semi-complex monomer, petro | 8 | Penalty | No specific examples – extrapolated from closest chemical analogues | Estimate including starting materials; polymerization is generally low in waste generation |
| Polymer, commodity monomer, renewable via chemical synthesis | 4 |  | No specific examples – extrapolated from closest chemical analogues | Estimate including starting materials and assuming valorization / recycling of waste biomass |
| Polymer, semi-complex monomer, renewable via chemical synthesis | 9 |  | ~0-2.26 (34 literature calculations; many only assessing polymerization step; optimized & non-optimized process; starting materials production excluded)27, 35 | Estimate including starting materials and assuming valorization / recycling of waste biomass |
| Biological material, direct use | 1 | Bonus | No specific examples | Assuming valorization / recycling or waste biomass; any waste would be essentially incidental (*e.g.*, fertilizer runoff) |
| Biological derivative, minimally refined | 2 | Bonus | 0.224-1.67 (2 literature calculations; optimized processes)19 | Estimate including starting materials and assuming valorization / recycling of waste biomass; waste due to refining |
| Biological derivative, moderately to highly refined | 5 |  | 45.7-88.9 (6 literature calculations; optimized & non-optimized process; biomass + solvents not recycled or valorized; initial feedstock processing excluded)19, 36, 37 | Estimate including starting materials and assuming valorization / recycling of waste biomass and extraction solvents; waste due to refining |
| Biological derivative, refined and chemically modified | 8 |  | 3.4-18.9 (16 literature calculations; optimized & non-optimized process; calculation parameters vary)38-40 | Estimate including starting materials and assuming valorization / recycling of waste biomass and extraction solvents. Assuming sum of refined bio derivative + renewable commodity chemical via chemical synthesis. |
| Ferment, direct use | 3 | Bonus | No specific examples – extrapolated from closest chemical analogues | Assume slightly better than commodity chemical via fermentation as no extraction is performed |

**Table S5.** EQ-factor model categories, values, underlying literature and supplier data, and commentary on expert judgement based value assignments for inorganics categories.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Component Category** | **E-Factor** | **“Q” Adjustment** | **Underlying Source Data** | **Commentary** |
| Sea salt | 1 | Bonus | *Via* seawater evaporation; less soluble salts are removed; salt is washed41 | Estimate including less soluble salt and contaminant removal |
| Salt, brine mined | 2 | Penalty | Isolation *via* heat, vacuum evaporation; chemical treatment to remove less soluble salts41 | Estimate including less soluble salt removal and refining / processing of brine; processing is hazardous |
| Sodium hydroxide | 3 | Penalty | Chloralkali process from NaCl (e-factor of balanced equation = 0.913) generates stoichiometric chlorine gas and hydrogen42, 43 | Hazardous byproduct generation |
| Potassium hydroxide | 3 | Penalty | *Via* electrolysis of KCl (analogous to chloralkali process; e-factor of balanced equation = 0.65); KCl from brine mining44, 45 | Hazardous byproduct generation |
| Organic potassium derivatives | 7 | Penalty | See Table S6. |  |
| Talc | 5 | Penalty | *Via* open pit rock mining; significant processing needed46, 47 | Assuming similar waste generation footprint as iron oxides; hazardous byproduct generation |
| Silica | 2 |  | *Via* open pit mining or dredging; calculated e-factor of processing = 1.3 (including tailings)8, 48, 49 | Very little literature data available |
| Silicone / siloxane / silane | 17 | Penalty | Silanol synthesis from silicon chlorides & siloxane bond synthesis generate multiple units HCl; further polymerization to cyclic siloxanes then linear silicones generate multiple units of H2O & CO2; further organic modification to complex silicones generate additional stoichiometric byproducts8, 50, 51 | Estimate including starting materials; ultra fine particle size quartz sand needed for silicone production (refining to obtain correct size); siloxane production is generally less efficient than traditional petrochemical reactions; hazardous byproduct generation |
| Mica | 1 |  | *Via* open pit or rock mining; little refining is performed52 | Assuming similar to silica mining but with less intensive processing |
| Kaolin Clay | 4 |  | *Via* open pit mining, hydraulic mining, or dredging; more intensive processing *versus* the other clays53 | Assuming twice as large waste impact as silica mining |
| Bentonite/ illite/ montmorillonite clay | 3 |  | *Via* open pit mining; physical and chemical processing / refining steps53 | Assuming similar to silica mining but with more intensive processing |
| Bentone gel (non-silicone) | 15 | Penalty | See Table S6. |  |
| Hectorite clay | 3 |  | *Via* open pit mining54 | Assuming similar to bentonite mining |
| Magnesium aluminum silicate | 3 |  | Mixture of natural clays (saponites and montmorillonites)55 | Assuming similar to bentonite mining |
| Iron oxide pigment | 5 |  | *Via* rock mining; can be byproduct of other metal refining processes; natural (minimal processing) and synthetic (extensive processing) pigments can be produced; calculated e-factor of iron ore processing = 3.1 (including tailings) 8, 56, 57 | Assuming additional processing steps are efficient; iron is extremely high volume commodity |
| Chromium oxide pigment | 8 | Penalty | Chromite *via* rock mining; oxides via thermal decomposition of chromic anhydride or reduction of sodium dichromate with ammonia sulfate; calculated e-factor of chromium ore processing = 5.7 (including tailings)8, 58-60 | Assuming additional processing steps are efficient; processing is hazardous |
| Ferric ferrocyanide | 6 |  | *Via* oxidation of ferrous ferrocyanide salts or reaction of iron with metallic cyanides61, 62 | Assuming slightly worse than iron oxides production waste impact |
| Inorganic magnesium derivatives | 3 |  | *Via* mining from salt deposits, brine mining with further refining, or reaction of magnesium carbonate (from thermal treatment of magnesite ore) or MgOH (from seawater) with sulfuric acid63, 64 | Assuming similar impact to sodium hydroxide  Though pure magnesium metal *via* rock mining has a calculated e-factor of 10 (including tailings), this was considered an overestimate *versus* inorganic derivatives production |
| Organic magnesium derivatives | 6 |  | See Table S6. |  |
| Calcium Carbonate | 3 |  | *Via* limestone refining65, 66 | Assuming similar impact to the clays |
| Organic calcium derivatives | 6 |  | See Table S6. |  |
| Inorganic calcium derivatives | 4 |  | Calcium silicate example *via* reaction of lime with silicates67, 68 | Assuming additional processing steps are efficient |
| Aluminum powder | 5 |  | *Via* rock mining; calculated e-factor = 4.2 (including tailings)8 |  |
| Inorganic aluminum derivatives | 6 | Penalty | Chlorine containing derivatives entail hazardous processing conditions69 | Assuming additional processing steps are efficient; aluminum is extremely high volume commodity |
| Organic aluminum derivatives | 9 |  | See Table S6. |  |
| Inorganic boron derivatives | 5 |  | Boron nitride example *via* nitridation of oxygen containing borates like boric acid or borax; borates *via* rock or brine mining with further refining70, 71 | Assuming similar impact to iron oxides production |
| Inorganic bismuth derivatives | 3 | Penalty | Bismuth is generally a refining byproduct of other metal ores, especially lead; bismuth oxychloride example *via* reaction of NaCl and bismuth salt72, 73 | Lead is highly hazardous; additional processing would not contribute significantly to e-factor as bismuth molecular weight is extremely high |
| Phosphoric acid | 8 | Penalty | Processing of phosphate ore is highly intensive; phosphogypsum byproduct is highly hazardous74-76 | Assuming similar waste impact to chromium; hazardous byproduct generation |
| Organic phosphate derivatives | 9 | Penalty | See Table S6. |  |
| Zinc oxide | 23 | Penalty | *Via* rock mining; zinc tailings are highly hazardous as zinc is generally mined with lead; calculated e-factor = 21 (including tailings)8, 77-81 | Assuming additional processing is efficient; hazardous byproduct generation |
| Organic zinc derivatives | 10 | Penalty | See Table S6. |  |
| Titanium dioxide | 4 | Penalty | Via rock mining; high volume of tailings produced; tailings are generally non-hazardous so not considered waste; calculated e-factor = 2.1; processing entails use of chlorine gas8, 82-84 | Ore processing entails high hazard |

**Table S6.** Calculated E-factors for specific convergent syntheses, with commentary on expert judgement based assumptions. MW, molecular weight.

|  |  |  |  |
| --- | --- | --- | --- |
| **Component Category** | **Assessed Chemical** | **Underlying Source Data and Calculations** | **Commentary** |
| Organic potassium derivatives | Potassium sorbate | MW of potassium sorbate is 150.1; MW of potassium is 39; MW of sorbic acid anion is 111.1; reaction of KOH and sorbic acid (semi complex, petro); calculated e-factor = 5.96.85 | Conservative category estimate of 7 based on this calculation |
| Bentone gel (non-silicone) | General Bentone gel | Various compositions are available; combination of bentonite and petro fine chemical. | Conservative category estimate of 15 based on petrochemistry e-factor |
| Organic magnesium derivatives | Magnesium stearate | MW of magnesium stearate is 307.8; MW of magnesium is 24.3; MW of stearic acid anion is 283.5; reaction of magnesium sulfate and stearic acid (moderately to highly refined biological derivative); calculated e-factor = 4.84. | Conservative category estimate of 6 based on this calculation |
| Organic calcium derivatives | Calcium stearate | MW of calcium stearate is 323.6; MW of calcium is 40.1; reaction of calcium oxide (from calcium carbonate, e-factor of balanced equation is 0.786) and stearic acid; calculated e-factor is 4.65; calculated e-factor of both reactions = 5.44.86, 87 | Conservative category estimate of 6 based on these calculations |
| Organic aluminum derivatives | General derivative | Derivatives of variable composition; combination of inorganic aluminum derivative and semi-complex, renewable via chemical synthesis. | Salt waste produced; conservative category estimate of 9 |
| Organic phosphate derivatives | General derivative | Derivatives of variable composition; combination of phosphoric acid and semi-complex, renewable via chemical synthesis. | Salt waste produced; conservative category estimate of 9 |
| Organic zinc derivatives | Zinc stearate | MW of zinc stearate is 348.9; MW of zinc is 65.4; reaction of zinc and stearic acid; calculated e-factor = 8.37. | Conservative category estimate of 10 based on this calculation |

# 6. Overview of OECD biodegradability test standards

**Table S7.** Overview of OECD test standards for biodegradability and environmental fate, highlighting the tiered screening approach.88

|  |  |  |  |
| --- | --- | --- | --- |
| **Biodegra-dability Test Tier** | **OECD Test Name** | **Pass Requirement** | **Notes** |
| Ready | 301A | >70% degradation in 28 days | - Ready tests are most stringent; all variants are conducted under aerobic conditions with a high test substance concentration (2-100 mg/L).  - Biodegradation rate is measured by non-specific parameters: *e.g.*, dissolved organic carbon (DOC), biochemical oxygen demand (BOD), carbon dioxide generation (CO2).  - All variants (excluding 301C) require relevant substances to pass a 10-day window, wherein the test pass level must be achieved within 10 days of the start of degradation (taken as the time at which 10% degradation has been achieved).  - A positive result on all tests can be considered indicative of rapid, ultimate degradation in most environmental conditions, including biological sewage treatment plants.  - Substances that fail the 10-day window but reach the test ‘pass’ level can be considered as inherently (ultimately) biodegradable. |
| 301B | >60% degradation in 28 days |
| 301C | >60% degradation in 28 days |
| 301D | >60% degradation in 28 days |
| 301E | >70% degradation in 28 days |
| 301F | >60% degradation in 28 days |
| 310 | >60% degradation in 28 days |
| Inherent | 302A | >70% (ultimate) | - Inherent tests entail a longer exposure (up to 60 days) and lower test substance concentration, increasing the potential for biodegradation to occur.  - A positive result on all tests can ***only*** be considered indicative of inherent, ultimate degradation in most environmental conditions ***if*** the 70% rate threshold is met. |
| 302B | >70% (ultimate) |
| 302C | >70% (ultimate) |
| Simulation | 303A | N/A | - Simulation tests are generally performed on substances that do not meet ready or inherent criteria; tests are intended to investigate substance fate within different environmental compartments.  - Results can be used to determine a degradation rate, which can be compared against regulatory thresholds to determine if the substance is ‘persistent.’  - Studies must be carefully evaluated to determine if metabolites requiring further consideration are generated. |
| 303B | N/A |
| 314A-E | N/A |
| 309 | N/A |
| 308 | N/A |
| 307 | N/A |

References

1. M. J. Eckelman, M. S. Moroney, J. B. Zimmerman, P. T. Anastas, E. Thompson, P. Scott, M. McKeever-Alfieri, P. F. Cavanaugh and G. Daher, *Green Chemistry*, 2022, **24**, 2397-2408.

2. A. G. Parvatker and M. J. Eckelman, *ACS Sustainable Chemistry & Engineering*, 2019, **7**, 350-367.

3. Y. Gong, X. Zheng, G. Liu and K. L. Lam, *Water Research*, 2024, **255**, 121439.

4. B. Köck, A. Friedl, S. Serna Loaiza, W. Wukovits and B. Mihalyi-Schneider, *Sustainability*, 2023, **15**, 5531.

5. R. A. Sheldon, *Chemical Society Reviews*, 2012, **41**, 1437-1451.

6. J. K. Satyarthi, D. Srinivas and P. Ratnasamy, *Applied Catalysis A: General*, 2011, **391**, 427-435.

7. A. Mustafa, S. Faisal, I. A. Ahmed, M. Munir, E. P. Cipolatti, E. A. Manoel, C. Pastore, L. di Bitonto, D. Hanelt, F. O. Nitbani, Z. M. El-Bahy, A. Inayat, T. M. M. Abdellatief, K. Tonova, A. Bokhari and A. Abomohra, *Biotechnology Advances*, 2023, **69**, 108275.

8. N. T. Nassar, G. W. Lederer, J. L. Brainard, A. J. Padilla and J. D. Lessard, *Environmental Science & Technology*, 2022, **56**, 6710-6721.

9. R. A. Sheldon, M. L. Bode and S. G. Akakios, *Current Opinion in Green and Sustainable Chemistry*, 2022, **33**, 100569.

10. M. O. Guerrero-Pérez and M. A. Bañares, *Catalysis Today*, 2015, **239**, 25-30.

11. M. Uyttebroek, W. Van Hecke and K. Vanbroekhoven, *Catalysis Today*, 2015, **239**, 7-10.

12. A. R. C. Morais, S. Dworakowska, A. Reis, L. Gouveia, C. T. Matos, D. Bogdał and R. Bogel-Łukasik, *Catalysis Today*, 2015, **239**, 38-43.

13. G. Juodeikiene, D. Vidmantiene, L. Basinskiene, D. Cernauskas, E. Bartkiene and D. Cizeikiene, *Catalysis Today*, 2015, **239**, 11-16.

14. J. P. M. Sanders and R. A. Sheldon, *Catalysis Today*, 2015, **239**, 44-49.

15. A. Marinas, P. Bruijnincx, J. Ftouni, F. J. Urbano and C. Pinel, *Catalysis Today*, 2015, **239**, 31-37.

16. J. M. Pinazo, M. E. Domine, V. Parvulescu and F. Petru, *Catalysis Today*, 2015, **239**, 17-24.

17. E. V. Ovchinnikova, G. F. Mironova, S. P. Banzaraktsaeva, E. A. Skiba, V. V. Budaeva, M. A. Kovgan and V. A. Chumachenko, *ACS Sustainable Chemistry & Engineering*, 2021, **9**, 16588-16596.

18. D. R. G. de Faria, J. L. de Medeiros and O. d. Q. F. Araújo, *Journal of Environmental Management*, 2021, **300**, 113772.

19. A. Schonhoff, N. Ihling, A. Schreiber and P. Zapp, *ACS Sustainable Chemistry & Engineering*, 2022, **10**, 9345-9358.

20. R. Parate, M. Borgave, M. Dharne and C. Rode, *Journal of Chemical Technology & Biotechnology*, 2021, **96**, 1316-1325.

21. A. D. Patel, S. Telalović, J. H. Bitter, E. Worrell and M. K. Patel, *Catalysis Today*, 2015, **239**, 56-79.

22. G. Pradhan and Y. C. Sharma, *Journal of Cleaner Production*, 2021, **315**, 127860.

23. A. Kuznetsov, G. Kumar, M. A. Ardagh, M. Tsapatsis, Q. Zhang and P. J. Dauenhauer, *ACS Sustainable Chemistry & Engineering*, 2020, **8**, 3273-3282.

24. E. Papadakis, PhD Thesis, Technical University of Denmark, 2016.

25. P. J. Dunn, S. Galvin and K. Hettenbach, *Green Chemistry*, 2004, **6**, 43-48.

26. F. Roschangar, R. A. Sheldon and C. H. Senanayake, *Green Chemistry*, 2015, **17**, 752-768.

27. S. Fadlallah, P. Sinha Roy, G. Garnier, K. Saito and F. Allais, *Green Chemistry*, 2021, **23**, 1495-1535.

28. T. V. T. Phan, C. Gallardo and J. Mane, *Green Chemistry*, 2015, **17**, 2846-2852.

29. F. Tieves, F. Tonin, E. Fernández-Fueyo, J. M. Robbins, B. Bommarius, A. S. Bommarius, M. Alcalde and F. Hollmann, *Tetrahedron*, 2019, **75**, 1311-1314.

30. P. Domínguez de María, *Current Opinion in Green and Sustainable Chemistry*, 2021, **31**, 100514.

31. D. Grajales-Hernández, M. Armendáriz-Ruiz, S. Velasco-Lozano, F. López-Gallego and J. C. Mateos-Díaz, *Applied Microbiology and Biotechnology*, 2020, **104**, 10033-10045.

32. N. Boaz and S. Clenennen, A Green, Solvent-free Biocatalytic Method to Produce Cosmetic Esters, <https://www.cosmeticsandtoiletries.com/research/methods-tools/article/21837041/a-green-solvent-free-biocatalytic-method-to-produce-cosmetic-esters>, (accessed June 4, 2022).

33. S. R. Madabhushi, N. D. S. Pinto and H. Lin, *New Biotechnology*, 2022, **72**, 122-127.

34. S. Fadlallah, A. L. Flourat, L. M. M. Mouterde, M. Annatelli, A. A. M. Peru, A. Gallos, F. Aricò and F. Allais, *Macromolecular Rapid Communications*, 2021, **42**, 2100284.

35. D. Winfield, J. Ring, J. Horn, E. M. White and J. Locklin, *Green Chemistry*, 2021, **23**, 9658-9668.

36. R. Mel and M. Malalgoda, *Cereal Chemistry*, 2022, **99**, 21-36.

37. R. Kisanthia, A. J. Hunt, J. Sherwood, L.-o. Somsakeesit and C. Phaosiri, *ACS Sustainable Chemistry & Engineering*, 2022, **10**, 104-114.

38. K. N. Onwukamike, S. Grelier, E. Grau, H. Cramail and M. A. R. Meier, *ACS Sustainable Chemistry & Engineering*, 2019, **7**, 1826-1840.

39. Natural, Sustainable Innovation: L'Oreal's Commitment to Renewable Materials & Eco-friendly Processes, <https://www.acs.org/content/dam/acsorg/events/popular-chemsitry/Slides/2017-02-16-cosmetics-slides.pdf>, (accessed June 1, 2022).

40. A. Cavezza, C. Boulle, A. Guéguiniat, P. Pichaud, S. Trouille, L. Ricard and M. Dalko-Csiba, *Bioorganic & Medicinal Chemistry Letters*, 2009, **19**, 845-849.

41. Salt Manufacture, <https://www.britannica.com/science/salt/Salt-manufacture>, (accessed June 1, 2022).

42. F. Du, D. M. Warsinger, T. I. Urmi, G. P. Thiel, A. Kumar and J. H. Lienhard V, *Environmental Science & Technology*, 2018, **52**, 5949-5958.

43. J. Crook and A. Mousavi, *Environmental Forensics*, 2016, **17**, 211-217.

44. H. Schultz, G. Bauer, E. Schachl, F. Hagedorn and P. Schmittinger, in *Ullmann's Encyclopedia of Industrial Chemistry, Volume 30*, eds. M. Bohnet, J. Brinker and B. Cornils, Wiley-VCH, Weinheim, Germany, 6 edn., 2000, DOI: <https://doi.org/10.1002/14356007.a22_039>.

45. Mineral Commodity Summaries 2022, <https://pubs.usgs.gov/periodicals/mcs2022/mcs2022.pdf>, (accessed December 5, 2022).

46. AP-42, Fifth Edition, Volume I Chapter 11.26: Talc Processing, <https://www3.epa.gov/ttnchie1/ap42/ch11/final/c11s26.pdf>, (accessed June 4, 2022).

47. H. King, Talc: The Softest Mineral, <https://geology.com/minerals/talc.shtml>, (accessed June 2, 2022).

48. Silica Statistics and Information, <https://www.usgs.gov/centers/national-minerals-information-center/silica-statistics-and-information>, (accessed June 1, 2022).

49. S. Platias, K. I. Vatalis and G. Charalampides, *Procedia Economics and Finance*, 2014, **14**, 491-498.

50. H. Sakurai, in *Encyclopedia of Inorganic Chemistry, Volume 8*, ed. R. B. King, John Wiley & Sons, Ltd, Hoboken, NJ, USA, 2 edn., 2006, DOI: <https://doi.org/10.1002/0470862106.ia220>.

51. L. Rösch, P. John and R. Reitmeier, in *Ullmann's Encyclopedia of Industrial Chemistry, Volume 32*, eds. M. Bohnet, J. Brinker and B. Cornils, Wiley-VCH, Weinheim, Germany, 6 edn., 2000, DOI: <https://doi.org/10.1002/14356007.a24_021>.

52. Mica, <https://mineralseducationcoalition.org/minerals-database/mica/>, (accessed June 2, 2022).

53. AP-42, Fifth Edition, Volume I Chapter 11.25: Clay Processing, <https://www.epa.gov/air-emissions-factors-and-quantification/ap-42-fifth-edition-volume-i-chapter-11-mineral-products-0>, (accessed June 10, 2022).

54. Chemistry and Properties of Bentone Hectorite Clay Based Rheology Modifiers, <https://www.elementis.com/fileadmin/elementis/About_Elementis/03-businesses/Performance_Specialties/Adding_Future/Papers_Leaflets/bentone/0102010302_Hectorite_BENTONE_Part_1_mineralogy.pdf>, (accessed June 3, 2022).

55. T. Pongjanyakul and S. Puttipipatkhachorn, *AAPS PharmSciTech*, 2009, **10**, 346-354.

56. A. Brioche, 2018 Minerals Yearbook: Iron Oxide Pigments, <https://d9-wret.s3.us-west-2.amazonaws.com/assets/palladium/production/atoms/files/myb1-2018-feoxi.pdf>, (accessed June 3, 2022).

57. Iron Oxide Pigments Statistics and Information, <https://www.usgs.gov/centers/national-minerals-information-center/iron-oxide-pigments-statistics-and-information>, (accessed June 2, 2022).

58. *US Pat.,* US4067747A, 1975.

59. H.-B. Xu, Y. Zhang, Z.-H. Li, S.-L. Zheng, Z.-K. Wang, T. Qi and H.-Q. Li, *Journal of Cleaner Production*, 2006, **14**, 211-219.

60. P. Li, H.-B. Xu, S.-L. Zheng, Y. Zhang, Z.-H. Li and Y.-L. Bai, *Environmental Science & Technology*, 2008, **42**, 7231-7235.

61. H. G. Völz, J. Kischkewitz, P. Woditsch, A. Westerhaus, W.-D. Griebler, M. De Liedekerke, G. Buxbaum, H. Printzen, M. Mansmann, D. Räde, G. Trenczek, V. Wilhelm, S. Schwarz, H. Wienand, J. Adel, G. Adrian, K. Brandt, W. B. Cork, H. Winkeler, W. Mayer, K. Schneider, L. Leitner, H. Kathrein, E. Schwab, H. Jakusch, M. Ohlinger, R. Veitch, G. Etzrodt, G. Pfaff, K.-D. Franz, R. Emmert, K. Nitta, R. Besold and H. Gaedcke, in *Ullmann's Encyclopedia of Industrial Chemistry, Volume 26*, eds. M. Bohnet, J. Brinker and B. Cornils, Wiley-VCH, Weinheim, Germany, 6 edn., 2006, DOI: <https://doi.org/10.1002/14356007.a20_243.pub2>.

62. A. V. Vyboishchik and M. Y. Popov, *IOP Conference Series: Materials Science and Engineering*, 2020, **962**, 022035.

63. *WIPO (PCT) Pat.,* WO2013037649A1, 2011.

64. M. Rao, Magnesium Sulfate, <https://www.fao.org/fileadmin/templates/agns/pdf/jecfa/cta/68/Magnesium_Sulfate.pdf>, (accessed June 6, 2022).

65. G. Crapper, in *Polymer Science: A Comprehensive Reference, Volume 10*, eds. K. Matyjaszewski and M. Möller, Elsevier, Amsterdam, 2012, DOI: <https://doi.org/10.1016/B978-0-444-53349-4.00279-X>, pp. 541-566.

66. *US Pat.,* US6251356B1, 1999.

67. N. Betancur Granados, J. Tobón and O. Restrepo, *Civil Engineering Research Journal*, 2018, **5**, 555665.

68. J. P. Ingham, in *Geomaterials Under the Microscope*, ed. J. Northcott, Manson Publishing Ltd., London, U.K., 2013, DOI: <https://doi.org/10.1016/B978-0-12-407230-5.50014-5>, ch. 6, pp. 121-127.

69. *US Pat.,* US4267161A, 1980.

70. Final Summary Report of Mineral Industry Processing Wastes, <https://nepis.epa.gov/Exe/ZyPURL.cgi?Dockey=P1005N9Y.TXT>, (accessed June 3, 2022).

71. E. Burcu, in *Sintering Applications*, ed. E. Burcu, IntechOpen, Rijeka, Croatia, 2013, DOI: 10.5772/53325, ch. 2.

72. *China Pat.,* CN102010003A, 2010.

73. S. Singerling and R. Callaghan, 2018 Minerals Yearbook: Bismuth, <https://pubs.usgs.gov/myb/vol1/2018/myb1-2018-bismuth.pdf>, (accessed June 7, 2022).

74. Energy and Environmental Profile of the U.S. Mining Industry: Phosphates, <https://www.energy.gov/sites/default/files/2013/11/f4/phosphate.pdf>, (accessed June 3, 2022).

75. G. Reta, X. Dong, Z. Li, B. Su, B. Huijuan, D. Yu, H. Wan, L. Ji, Y. Li, G. Xu, K. Wang and S. Xu, *International Journal of Hydrology*, 2018, **2**, 424-431.

76. Y. Taha, A. Elghali, R. Hakkou and M. Benzaazoua, *Minerals*, 2021, **11**, 1250.

77. Zinc, <https://www.ga.gov.au/education/classroom-resources/minerals-energy/australian-mineral-facts/zinc>, (accessed October 5, 2023).

78. P. Russel and T. Tharmanathan, Lead and Zinc, <https://uwaterloo.ca/wat-on-earth/news/lead-and-zinc>, (accessed October 5, 2023).

79. Z. Su, Q. Chen, Q. Zhang and D. Zhang, *Minerals*, 2019, **9**, 710.

80. J. Tenório Vinhal, R. Húngaro Costa, J. Luís Coleti and D. C. R. Espinosa, *The Canadian Journal of Chemical Engineering*, 2021, **99**, 166-177.

81. T. Gao, Q. Ji, G. Li and X. Zhu, *Journal of Physics: Conference Series*, 2023, **2520**, 012018.

82. Titanium, <https://www.ga.gov.au/education/classroom-resources/minerals-energy/australian-mineral-facts/titanium>, (accessed October 5, 2023).

83. D. M. Maina, D. M. Ndirangu, M. M. Mangala, J. Boman, K. Shepherd and M. J. Gatari, *Environ Sci Pollut Res Int*, 2016, **23**, 21431-21440.

84. M. J. Eckelman, J. B. Zimmerman and P. T. Anastas, *Journal of Industrial Ecology*, 2008, **12**, 316-328.

85. *US Pat.,* US4639294A, 1987.

86. Calcium Stearate Processing, <https://www.ams.usda.gov/sites/default/files/media/Calcium%20Stearate%20TR.pdf>, (accessed June 2, 2022).

87. *US Pat.,* US3991172A, 1974.

88. OECD Guidelines for the Testing of Chemicals, Section 3, <https://doi.org/10.1787/2074577x>, (accessed September 18, 2023).