Data Selection Process for Formulas and Ingredients

Ingredients in PCP formulas were identified by the International Nomenclature of Cosmetic Ingredients (INCI) name, and in most cases, one or more associated Chemical Abstracts Service registry numbers (CASRNs). To estimate environmental impact, the chemical structure of the ingredient is necessary. Simplified molecular-input line-entry system (SMILES) structures were obtained using the US EPA CompTox Chemicals Dashboard internet database in batch mode with CASRNs as input. Missing structures were determined using other authoritative databases (e.g., Royal Society of Chemistry's ChemSpider, US NIH's CACTUS). For mixtures, we used sources describing the component chemical structures including manufacturers' documentation available on UL Prospector and European Chemicals Agency internet databases.

The tool was constructed to automatically use the results of quantitative structure activity relationship (QSAR) models as a default, and the QSAR-generated data can be overwritten manually during subsequent empirical data curation efforts. We selected two US EPA QSAR software packages to initially populate the tool: TEST Version 5.1.1 and EPISuite Version 4.11. For all values except the fish bioconcentration factor (BCF), when both TEST and EPISuite provided an estimate, the TEST results were preferentially used and EPISuite results filled data gaps left by TEST. We implemented this priority scheme in reverse for BCF, using the Arnot-Gobas Upper Trophic estimate preferentially. TEST results were directly used in the tool. We programmed the tool to extract empirical and modeled data from EPISuite's output reports. Many QSARs rely on the octanol-water partition coefficient, which is not meaningful for surfactants due to surface activity and micelle formation, so we superseded model results with empirical data for ecotoxicity values for surfactants. We identified surface active substances using the EU Cosmetics Ingredients (CosIng) internet database, where "surfactant" is identified as a functional category for surface active PCP ingredients.

For polymers and inorganic substances, predictive modeling options are limited, so a combination of empirical data and default values recommended for regulatory assessments were used, requiring a higher level of data curation. For mixtures of homologous compounds and substances of unknown or variable composition, complex reaction products or biological materials (UVCBs) where the major components were known a base-case ranking approach for one to three representative compounds were used and the poorest rank among them was adopted to represent the ingredient mixture's rank.

Deviations from Okonski et al. (2021) Method for PNEC Development

We implemented the method of Okonski et al. (2021) with the following changes to facilitate automation, though the unabridged method or a different approach for determining the PNEC, e.g., a species-sensitivity distribution, can be used by overriding the automatically calculated value. For pragmatism, a total of nine aquatic toxicity tests– three acute, three intermediate, and three chronic– is the maximum automatically considered for selection of the critical toxicity value rather than an unlimited number. For the few ingredients with more available data, additional data must be included manually. If no manual entry is made, the tool assumes there is one test result available for each trophic level, resulting in a more conservative AF and PNEC. The mode of action is assigned using output from the TEST or ECOSAR model as described in SI. Values for the Fmoa parameter are: 1 for narcosis, 5 for

non-narcosis, and guidance in the tool advises assigning a larger value if warranted (e.g., endocrine effects known but not captured in the data set).

Mode of Action Determination

The mode of action is assigned in the tool using the Fathead Minnow LC50 "Mode of Action" model in the TEST software package. For data gaps, the ECOSAR module of EPISuite was used. For substances with a mode of action listed as "Narcosis" (TEST) or only "Baseline" in ECOSAR, the Fmoa value (the mode of action portion of the AF) was assigned a value of one. If the mode of action in TEST was anything other than "Narcosis," or if ECOSAR suggested QSAR models besides baseline toxicity, or if there is no prediction in TEST or ECOSAR, the Fmoa value was set to 5. The tool suggests curation by the user to assign a higher value for Fmoa when warranted, e.g. in the case of endocrine disrupting compounds where the data set does not adequately capture endocrine effects.

Ecotoxicity in Sediment and Soil

Toxicity to sediment organisms is considered for non-readily biodegradable substances where the EPISuite Fugacity model predicts that ≥10% of the emitted mass would partition to sediment. The Fugacity model is run using default parameters, except with emissions to soil and air changed to zero (i.e., 100% of emissions to water). The 10% threshold was selected with reference to the EU Medicines Agency ERA guidelines (EMA, 2006), in which the sediment effects pathway is only considered if ≥10% of a medicinal substance partitions to sediment during laboratory simulation testing. Similarly, toxicity to soil organisms is considered for non-readily biodegradable substances where the EPISuite Sewage Treatment Plant (STP) model predicts that ≥10% of the emitted mass would partition to biosolids in STPs, hence potentially reach soil amended with biosolids as fertilizer. There is no "credit" given for loss of the substance to biosolids in the STP, reducing the proportion of the substance available to sediment, because this process varies among localities. In some areas, STPs only provide primary treatment, limiting the opportunity for partitioning losses during treatment, and in others with combined sewers, STP bypasses are common during wet weather events (Phillips et al, 2012). As a result, even though areas served by efficient STPs would have mitigated exposure in sediments; in other areas with less efficient STPs or frequent bypasses, sediment exposure would still occur.

Persistence of Non-Readily Biodegradable Substances

Non-readily biodegradable substances are evaluated for persistence in multiple media as follows: for all substances, by their half-life in water, and for substances that partition to sediment or soil ≥ 10% (as described in Section 3.2.1), also by their half-life in sediment and/or soil. As a default in the ranking tool, the US EPA EPISuite Fugacity model's method was used as the basis for assigning half-life values in water with two modifications: (1) the change recommended by Aronson et al. (2006) was used (i.e., BIOWIN result of "months" correlates to a duration of 120 days rather than the default value in EPISuite), and (2) rather than using discrete bins to relate BIOWIN 3 (ultimate biodegradation expert survey) model results to half-life values, a regression model was developed to create a continuous

function for determining the half-life in water from BIOWIN 3 output, shown in Table S4 – Derivation of Aqueous Half-Life Model. For sediment, the half-life is assumed to be the aqueous half-life multiplied by nine, and for soil, the half-life is assumed to be the aqueous half-life multiplied by 2, which are the default for these parameters in the Fugacity model (See Table S6 – Default Values and Practices).

Minor Ingredients Neglected in Product Ranks

The results in Tables S7 and S8 include 94.5% or more of the ingredients (dry weight basis), because the rank cannot be mathematically altered by a fraction of the formula less than 5.5%. Hence, the smallest components of each formula were neglected, leaving at least 94.5% of the total weight evaluated.

References

Phillips PJ, Chalmers AT, Gray L, Kolpin DW, Foreman WT, Wall GR. 2012. Combined Sewer Overflows: An Environmental Source of Hormones. Environ. Sci. Technol. 46:5336−5343. doi: 10.1021/es3001294

Example Calculation, Base-Case

Phenoxyethanol, CAS RN 122-99-6

Shaded tables show values from the tool's spreadsheet used to calculate the outcome

Ecotoxicity Sub-Rank Value Determination

PNEC calculation adapted from Okonski et al. 2021

Aquatic toxicity (E/M = empirical/modeled)

Acute values (mg/L)

Fish LC50	E/M	Source	Daphnia EC50	E/M	Source	Algae EC50	E/M	Source	SEV1
343.91	E	TEST	91.77	M	TEST	381.272	M	ECOSAR	9.177

Subchronic/intermediate values (mg/L)

Fish LC50	E/M	Source	Daphnia EC50	E/M	Source	Algae EC50	E/M	Source	SEV2

Chronic values (mg/L)

Fish ChV	E/M	Source	Daphnia ChV	E/M	Source	Algae ChV	E/M	Source	SEV3
64.663	M	ECOSAR	29.506	M	ECOSAR	43.843	M	ECOSAR	29.506

PNEC Determination

SEVf	CTV	Critical Species
9.177	91.77	Primary consumer

Fes	Fsv	MOA	Source	Fmoa	AF	PNECaq
10	5	Narcosis	TEST	1	50	1.835

Partitioning prediction from EPISuite STP and fugacity models

Water%	Sediment%	Soil%
99.134	0.207	0.667

% soil = % in sludge biosolids in STP model

% water, % sed = %water, %sed from EPI Suite fugacity model × (100% - % in biosolids)/100%

No adjustment made for STP biodegradation losses, because
some locales have poor STP removal or frequent wet weather bypasses

< 10% predicted in sediment --> no sediment PNEC needed

< 10% predicted in biosolids (sludge) --> no soil PNEC needed

Soil and Sediment PNEC (mg/kg) demonstration (not required for phenoxyethanol)

log Koc	E/M	Source
1.174	M	KOCWIN

$PNECsoil = PNECaq \times (0.01764 \times K_{oc} + 0.1176)$

$PNECsed = PNECaq \times (0.0217 \times K_{oc} + 0.783)$

PNECsoil	PNECsed
0.699	2.032

PNEC scaled to obtain Ecotoxicity Sub-rank Value (SRV)

SRVaq = 1.355 - 4.5 × log (PNECaq)

SRVsoil/sed = 6.274 - 2.726 × log (PNECsoil/sed)

overall SRV = minimum SRV (water, sediment, soil)

SRV ecotox
0.168

Persistence Sub-Rank Value Determination

Ready Biodegradability Prediction from US EPA BIOWIN model

BIOWIN3	BIOWIN 5	Ready Bio
3.0177	0.7974	Yes

If BIOWIN3 > 2.75 and BIOWIN5 > 0.5 then ready biodegradability prediction is "Yes"

Partitioning prediction from EPISuite STP and fugacity models

Water%	Sediment%	Soil%
99.134	0.207	0.667

% soil = % in sludge biosolids in STP model

% water, % sed = %water, %sed from EPI Suite fugacity model × (100% - % in biosolids)/100%

No adjustment made for STP biodegradation losses, because
some locales have poor STP removal or frequent wet weather bypasses

< 10% predicted in sediment --> no sediment half-life needed

< 10% predicted in biosolids (sludge) --> no soil half-life needed

Half-life values (demonstrated for all media, needed for water only in this case)

$t_{1/2aq}$ (d) = $4662.3 \times e^{(-1.916(BIOWIN3))}$

$t_{1/2soil}$ (d) = $2 \times t_{1/2aq}$

$t_{1/2sed}$ (d) = $9 \times t_{1/2aq}$

Water t1/2	Sed t1/2	Soil t1/2
14.373	129.357	28.746

Half-life scaled to obtain Persistence Sub-rank Value (SRV)

Readily Biodegradable or $t_{1/2}$ < 7 d --> SRVaq = 0

$t_{1/2}$ > 180 d --> SRVaq = 9

Otherwise --> SRVaq = 2.7735 ln($t_{1/2}$) - 5.8362

Raw SRVaq	Raw SRVsed	Raw SRVsoil
0	not used	not used

SRV contribution from each compartment (weighted SRV) = SRVcompartment x % in compartment/% considered
e.g., for water, weighted SRVaq = 0 x 99.135%/(99.135% + 0.207% + 0.667%)
% considered can be < 100% due to volatilization

Wtd SRVaq	Wtd SRVsed	Wtd SRVsoil
0	not used	not used

SRV persist
0

Bioaccumulation Potential Sub-Rank Value Determination

Check for ready biodegradability and molecular weight cutoff

Mol wt	Ready Bio
138.170	Yes

Bioaccumulation Potential SRV determination

If mol. wt. > 1000 OR readily biodegradable = "yes", SRV = 0

Otherwise, check fish bioconcentration factor (BCF)

BCF and decision criteria shown below, but not needed in this case because prediction is readily biodegradable

BCF	E/M	Source
2.438	M	EPI Suite

If BCF < 100, SRV = 0
If BCF > 5000, SRV = 9
Otherwise SRV = -10.5 + 5.258 × log (BCF)

SRV bioacc
0

Rarer Impacts SRV determination

Local Potential Impact, Subsurface Mobility

Check half-life in water
If $t_{1/2aq}$ < 60 d, PI-indicator is "No"
If $t_{1/2aq}$ ≥ 60 d, check water solubility (WS) and organic carbon partition coefficient (Koc)

Water t1/2
14.37

In this case, $t_{1/2aq}$ < 60 d, so PI-indicator is "No"
WS, Koc and decision criteria shown below, but not needed in this case

WS (mg/L)	E/M	Source	log Koc	E/M	Source
26695.94	E	TEST	1.19	M	EPI Suite

If WS < 0.15 mg/L or if log Koc > 4, PI-indicator is "No"
Otherwise, PI-indicator is "yes"

Local Potential Impact, Ground Level Photochemical Ozone Formation

Check normal boiling point (BP)
If BP ≤ 250 °C, check ReCiPe model photochemical ozone formation list or
MIR List produced by the California Air Resources Board (CARB)

BP degC	E/M	BP source
245.00	E	TEST

Phenoxyethanol is listed as a potential source of photochemical ozone by CARB
PI-indicator is "Yes"

Local Potential Impact, Eutrophication

Check SMILES structure for the presence of phosphorus

SMILES (Unique)
OCCOC1=CC=CC=C1

Phosphorus is not present so PI-indicator is "No"

Global Potential Impacts: Climate Change, Stratospheric Ozone Depletion

Check ReCiPe model to see if substance is on the list of greenhouse gases or ozone depleters
Phenoxyethanol is not on either list, so the PI-indicator is "No"

Global Potential Impact, Mineral Resource Deplation

Check SMILES structure for elements on the Crustal Scarcity Potentials (CSPs) from Arvidsson et al. (2021)
Include all with a value > CSP for Zn, but excluding N
Phenoxyethanol does not include any minerals on the list, so the PI-indicator is "No"

Totals for Rarer Potential Impacts

0 global potential impacts, 1 local potential impact
For one local impact, SRV = 4, for two or more local impacts, SRV = 9
For one or more global impacts, SRV = 9

SRV rarer
4

Final Rank Determination

All SRV values are incremented by one for presentation to end users, changing from a scale of 0-9 to a scale of 1-10

SRV ecotox	SRV persist	SRV bioacc	SRV rarer
1	1	1	5

Multiply SRVs by weighting factors and round to a whole number to achieve final ingredient rank

Eco wt	Persist wt	Bioacc wt	Rarer wt
30%	30%	20%	20%

Final rank
2

Table S1 Weighting Factors

Outcome	Variables or Parameters Used	Weight Value Used	Reason
Final Rank Value - Base Case	Toxicity	30%	Identified as important impact category in shampoo life cycle assessment
	Bioaccumulation	20%	Global endpoint of concern; impacts sensitive top predators and difficult to reverse
	Persistence	30%	Pre-requisite for all adverse effects; Surrogate for unanticipated adverse effects to ecosystems
	Rarer Impacts Cluster	20%	Less common; grouped because considering separately creates rankings with less sensitivity
	Soil Mobility	Decrements Cluster Sub-Rank by 5	Impact dependent on local environment's susceptibility
	Ground-Level Photochemical Ozone (Smog)	Decrements Cluster Sub-Rank by 5	Impact dependent on local environment's susceptibility
	Eutrophication	Decrements Cluster Sub-Rank by 5	Impact dependent on local environment's susceptibility
	Climate Change (Direct Greenhouse Gas Emission)	Decrements Cluster Sub-Rank by 10	Global impact
	Stratospheric Ozone Depletion (Direct Emission)	Decrements Cluster Sub-Rank by 10	Global impact
	Mineral Resource Depletion	Decrements Cluster Sub-Rank by 10	Global impact
	Other	User-determined based on impact	Can be local or global depending on nature of the impact identified
Final Rank Value - Polymer	Rank Value - Polymer	70%	Relatively high uncertainty about degradation mechanisms, rate, and risk from fragments, so weight is
	Rank Value - Polymer Fragment of Concern	30%	biased more heavily toward the Rank Value of the emitted substance
Final Rank Value - Inorganic/Organometallics			
Case 1: Rapidly and Completely Dissociates	Rank Value - Inorganic/Organometallic	0%	The substance listed on the label dissociates completely in the product or immediately after use in water, so
	Rank Value - Metal of Concern	100%	only the transformation products are relevant (e.g., NaOH used for pH adjustment)
Case 2: Measureable Dissociation	Rank Value - Inorganic/Organometallic	70%	Less uncertainty about transformation and risk of transformation products, but rate of dissolution is
	Rank Value - Metal of Concern	30%	extremely slow, mitigating risk
Case 3: No Measureable Dissociation	Rank Value - Inorganic/Organometallic	90%	Less uncertainty about transformation and risk of transformation products, but rate of dissolution is
	Rank Value - Metal of Concern	10%	extremely slow, mitigating risk

Table S2 Assessment Triggers

Decision Triggered	Triggering Conditions	Actions Taken
Environmental fate-related		
Water pathway considered	All non-polymeric substances Anionic polymers unless empirical data indicates "insoluble" Other polymers if empirical data noes not indicate "insoluble"	Aquatic toxicity and persistence sub-ranks are included in the final rank value
Soil pathway considered	EPISuite STP model indicates ≥ 10% partitions to sludge	Soil toxicity and persistence sub-ranks are included in the final rank value
Sediment pathway considered	EPISuite Fugacity model indicates ≥ 10% partitions to sediment	Sediment toxicity and persistence sub-ranks are included in the final rank value
Persistence-related		
Bioaccumulation considered	All non-readily biodegradable substances	Bioaccumulation sub-rank is included in the final rank value
Subsurface Migration evaluation started	Substances with aqueous $t_{1/2}$ ≥ 60 days	Further subsurface mobility evaluation is triggered
Additional Impacts-Related		
Subsurface Migration determined	Water solubility ≥ 0.15 mg L^{-1}, *and* Log K_{oc} < 4	Impact of concern decision for Subsurface Mobility toggled to "Yes"
Eutrophication determined	Substance contains phosphorus	Impact of concern decision for Eutrophication toggled to "Yes"
Ground-Level Ozone formation determined	Boiling point ≤ 250 °C, *and* Substance is listed as photochemical ozone former on authoritative list	Impact of concern decision for Ground-Level Ozone Formation toggled to "Yes"
Direct Climate Change Emission determined	Substance is listed by ReCiPe model as contributing to climate change	Impact of concern decision for Direct Climate Change Emission toggled to "Yes"
Stratospheric Ozone Depletion determined	Substance is listed by ReCiPe model as contributing to stratospheric ozone depletion	Impact of concern decision for Stratospheric Ozone Depletion toggled to "Yes"
Mineral Resource Depletion determined	Substance includes mineral substance with scarcity ≥ zinc in life cycle impact approach of Arvidsson *et al.* (2020)	Impact of concern decision for Mineral Resource Depletion toggled to "Yes"
Other Issue determined	Unique or newly emerging intrinsic hazard not captured elsewhere is identified by assessor (*e.g.* , physical hazard)	Impact of concern decision for Other Issue toggled to "Yes"

Table S3 PNEC Derivation

Parameter	Data Type	Value Used	Implementation notes
Aquatic Assessment Factor Components			
Endpoint standardization factor (F_{ES})	Acute guideline study	10	
	Acute QSAR model result	10	TEST model L(E)C_{50} preferred; Otherwise ECOSAR L(E)C_{50}
	Suchronic study	5	
	Chronic guideline study	1	
	Chronic QSAR model result	1	ECOSAR ChV
Species variation factor (F_{SV})	One trophic level, one species in data set	50	
	One trophic level, 2-3 species in data set	20	
	One trophic level, 4-6 species in data set	10	
	One trophic level, 7+ species in data set	5	
	Two trophic levels, 1-2 species in data set	10	
	Two trophic levels, 3-5 species in data set	5	
	Two trophic levels, 6+ species in data set	2	
	Three trophic levels, 3 species in data set	5	
	Three trophic levels, 4-6 species in data set	2	
	Three trophic levels, 7+ species in data set	1	
Mode-of-action factor (F_{MOA})	Narcosis	1	TEST model prediction preferred; Otherwise, substances categorized only as "neutral organic" in ECOSAR
	Non-narcosis	5	TEST model prediction as non-narcotic preferred; Otherwise, substances categorized with models other than "neutral organic" in ECOSAR; Default for polymers
	High potency mode of action	50	Default value for substances with known potent toxicity (e.g., mammalian data showing endocrine disruption); Expected to be overridden manually in most cases based on empirical data
PNECs			
	Aquatic PNEC	Critical Toxicity Value / $F_{ES} \times F_{SV} \times F_{MOA}$	Critical Toxicity Value is determined according to the method of Okonski *et al.* (2021)
	Sediment PNEC with no sediment toxicity data	Aquatic PNEC × (0.0217 × K_{oc} + 0.783)	Equilibrium partitioning approach from REACH guidance (ECHA-11-G-16-EN p. 39)
	Sediment PNEC with sediment toxicity data	Critical Toxicity Value / Sediment AF	Selected manually by the assessor, using REACH guidance
	Soil PNEC with no soil toxicity data	Aquatic PNEC × (0.01764 × K_{oc} + 0.1176)	Equilibrium partitioning approach from REACH guidance (ECHA-11-G-16-EN p. 39)
	Soil PNEC with soil toxicity data	Critical Toxicity Value / Soil AF	Selected manually by the assessor, using REACH guidance

Table S4. Derivation of Aqueous Half-Life Model

Description	BIOWIN 3 Result Range		Result Value	Recommended	Regressed
	High value	Low value	Regressed	$t_{1/2}$ (d)[a]	$t_{1/2}$ (d)[b]
Recalcitrant	1.75		1.5	180	263.3
Months	2.25	1.75	2	120	101.0
Weeks to months	2.75	2.25	2.5	37.5	38.8
Weeks	3.25	2.75	3	15	14.9
Days to weeks	3.75	3.25	3.5	8.67	5.7
Days	4.25	3.75	4	2.33	2.2
Hours to days	4.75	4.25	4.5	1.25	0.8
Hours		4.75	5	0.17	0.3

Notes:

[a] Recommended in Aronson D, Boethling R, Howard P, Stiteler W. 2006. Estimating biodegradation half-lives for use in chemical screening. Chemosphere. 63:1953-1960.

[b] Regression model: $t_{1/2}(d) = 4662.3e^{-1.916(BIOWIN3)}$ $\left[R^2 = 0.94\right]$

Table S5 Scales Used to Assign Sub-Rank Values (SRVs) for the Ten Impact Categories

Parameter	Input Data Used	Sub-Rank Value (SRV)	Notes
Persistence			
Water	Readily biodegradable[a]	0	
	$t_{1/2}$ < 7 days	0	
	$t_{1/2}$ = 7 days	1	
	$t_{1/2}$ ≥ 180 days	9	
	7 d < $t_{1/2}$ < 180 days	2.7735 ln($t_{1/2}$) - 5.8362	Best fit equation to achive rank = 1 for $t_{1/2}$ = 7 d and rank = 9 for 180 d. Log relationship used to conform scale with PBT scales (i.e., rank increases rapidly then levels off with increasing $t_{1/2}$ to achieve poorer ranks with half-life near regulatory "P" thresholds)
Soil and Sediment	$t_{1/2}$ < 14 days	0	
	$t_{1/2}$ ≥ 180 days	9	
	14 d ≤ $t_{1/2}$ < 180 days	2.7668 ln($t_{1/2}$) - 7.351	Best fit equation to achive rank = 0 for $t_{1/2}$ = 14 d and rank = 9 for 365 d. Log relationship used to conform scale with PBT scales (i.e., rank increases rapidly then levels off with increasing $t_{1/2}$ to achieve poorer ranks with half-life near regulatory "P" thresholds)
Final Persistence Sub-Ranking	SRVs for all relevant media and % of substance in relevant media	(% in water × SRV_{water} + % in sediment × $SRV_{sediment}$ + % in soil × SRV_{soil}) / % in relevant compartments	SRV values are blank for media not relevant due to low partitioning, and those terms drop out from the calculation shown
Polymers	Readily biodegradable[a]	0	
	Inherently biodegradable	4	
	Not readily or inherently biodegradable or no data	9	
Inorganics	Sub-Rank Values for Toxicity, Bioaccumulation, and Other	0.44 × SRV_{TOX} + 0.28 × SRV_{BIOACC} + 0.28 × SRV_{RARE}	Peristence is considered essentially infinite; but effects are typically very well understood and persistence is only a concern to the degree that there are effects expected, so focus of Ranking shifts to the other impact categories, retaining the ratio between them in the 30%/20%/20% weighting scheme for Toxicity, Bioaccumulation, and Rarer Impacts
Ecological Toxicity			
Water	PNEC = 2 mg L^{-1}	0	Equivalent to a data set with three limits tests (*i.e.* , L(E)C_{50} ≥ 100 mg L^{-1}) for three trophic levels and three species
	PNEC = 0.02 mg L^{-1}	9	Equivalent to a data set of acute tests with three trophic levels and three species and a minimum L(E)C_{50} = 1 mg L^{-1}
	0.02 mg L^{-1} ≤ PNEC ≤ 2 mg L^{-1}	1.355 - 4.5 × log (PNEC)	Best fit equation to achieve rank = 0 for PNEC = 2 mg/L (this would occur when L(E)C_{50} ≥ 100 mg/L in tests for all three trophic levels in our PNEC derivation algorithm) and rank = 9 for PNEC = 0.02 mg/L (would occur for critical L(E)C_{50} = 1 mg/L with data from three trophic levels)
Soil and Sediment	PNEC = 200 mg kg^{-1}	0	Equivalent to aquatic PNEC = 2 mg L^{-1} and K_{oc} = 100 or aquatic PNEC = 0.02 mg L^{-1} and K_{oc} = 10,000
	PNEC = 0.1 mg kg^{-1}	9	Screening value in soil below which biologically potent active ingredients are not a concern in EMA veterinary guidance
	0.1 mg L^{-1} ≤ PNEC ≤ 200 mg L^{-1}	6.274 - 2.726 × log (PNEC)	Best fit equation to achieve rank = 0 for PNEC = 200 mg/L (this would occur when L(E)C_{50} ≥ 100 mg/L in tests for all three trophic levels in our PNEC derivation algorithm) and rank = 9 for PNEC = 0.1 mg/L (would occur for critical L(E)C_{50} = 1 mg/L with data from three trophic levels)
Final Toxicity Sub-Ranking	SRVs for all relevant media	Minimum (SRV_{water}, $SRV_{sediment}$, SRV_{soil})	
Bioaccumulation/Secondary Poisoning			
	Readily biodegradable[a]	0	
	Not readily biodegradable, *and*		
	BCF < 100	0	100 exempts a substance from PBT in GHS; 500 is "low level" of bioaccumulation in GHS
	BCF ≥ 5000	9	2000 is "B" and 5000 is "vB" in regulatory PBT assessment
	100 ≤ BCF < 5000	-10.5 + 5.258 log (BCF)	Best fit equation to achieve rank = 0 for BCF = 100, rank = 4 for BCF = 500, rank = 7 for BCF = 2000, and rank = 9 for BCF = 5000
Rare Impacts Cluster			
	"No" for all Additional Impacts	0	
	"Yes" for one local impact[b]	4	
	"Yes" for 2+ local impacts[b]	9	
	"Yes" for 1+ global impact(s)[c]	9	

Notes:

[a] Substances that meet all criteria for ready biodegradability except the 10-day window are considered readily biodegradable in this system

[b] Additional Impacts considered local in scale are: Subsurface Migration, Eutrophication, Ground-Level Photochemical Ozone (Smog) formation, and potentially Other Issue, depending on the impact

[c] Additional Impacts considered global in scale are: Mineral Resource Depletion, Direct Climate Change Emission, and potentially Other Issue, depending on the impact

Table S6. Default Values and Practices

Parameter	Default Value When No Available Data	Notes
Polymers		US EPA TSCA:[a] "Rules of thumb are available to inform judgments about [environmental fate] processes [for polymers], but in general they are based on a heavy dose of faith and relatively few data." The dearth of data available to for polymer ERA has changed little since that was written.[b]
Log K_{oc}	4	US EPA TSCA "polymers will tend to partition to soil, suspended particles, sediments and sludge"[a]
Volatility	negligible	US EPA TSCA: vapor pressure and Henry's Law constant < 10^{-8} mm Hg assumed[a]
Water solubility	for non-neutral polymers or reported as "soluble," WS = 1000 mg/L otherwise 0 mg/L	Source: US EPA TSCA[a]
Partitioning	for soluble/dispersible anionic polymers with MW < 5000 Da, water only; for all else, water, sediment, and soil considered	Source: US EPA TSCA[a]
BCF	for MW > 1000 Da, BCF = 100	Source: US EPA TSCA[a]
Biodegradability	Slow	Source: US EPA TSCA[a]
Subsurface mobility	"Yes" if not readily biodegradable and water soluble/dispersible > 0.15 mg/L	In contrast to US EPA TSCA:[a] "for polymers it is generally assumed that releases to landfills and deep well injection do not result in significant aquatic- or terrestrial-ecological exposures" to reflect changes in thinking driven by PFAS issues
Aquatic toxicity	Negligible (Ecotoxicity sub-rank = 1) if "insoluble" regardless of charge; Read-across to closest structural analog for water soluble/dispersible polymers	Source: US EPA TSCA[a]
Identity of fragment of concern	Monomer	If a specific fragment is a known concern, this used; For chemically complex polymers, several potential fragments of concern can be ranked and the poorest rank used
Rare Impacts	"No"	Assumed that no significant impact exists if evidence is not found in sources selected (See Table S2. Assessment Triggers)
Sediment $t_{1/2}$	9 × Water $t_{1/2}$	US EPA default in EPISuite
Soil $t_{1/2}$	2 × Water $t_{1/2}$	US EPA default in EPISuite
Rounding	Only for final sub-ranks and ranks presented to the end-user	Sub-rank values are not rounded to whole numbers before calculation of final rank value, but sub-rank values are rounded for presentation to end-user
Bioaccumulation sub-rank for essential metals	0 (best)	BCF values are not indicative, because organisms regulate the internal concentration of essential metals, which can appear as bioaconcentration in some circumstances

Notes

[a] Sources: Nabholz, V. Undated. P2 Assessment of Polymers A Discussion of Physical-Chemical Properties, Environmental Fate, Aquatic Toxicity, and Non-Cancer Human Health Effects of Polymers. Available (2 August 2021) at: https://www.epa.gov/sites/default/files/2015-05/documents/07-assessmentpolymers.pdf and Boethling RS, Nabholz JV. 1996. Environmental Assessment of Polymers Under the U.S. Toxic Substances Control Act. Available (2 August 2021) at: https://nepis.epa.gov/

[b] Source: European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC). 2019. The ECETOC Conceptual Framework for Polymer Risk Assessment (CF4Polymers). Technical Report No. 133-1. Brussels, May. ISSN-2079-1526-133-1

Table S7 Ranking Results for Ten Shampoo Products

		Shampoo Product Name and Composition (Dry % w/w)									
INCI Name	**Rank**	**Children's**	**Revitalizing**	**Men's**	**Men's Dandruff**	**Hair & Body**	**Post-Treatment**	**Color Protect**	**Color Correct**	**Bar**	**PEFCR Model Shampoo**
Acrylates Copolymer	3	-	-	-	2.6	-	-	-	-	-	-
Acrylates/C10-30 Alkyl Acrylate Crosspolymer	3	-	4.0	-	-	-	-	-	-	-	-
Agar	3	-	-	-	-	-	-	-	-	15.7	-
Ammonium Laureth Sulfate	4	-	-	-	-	-	-	29.6	-	-	-
Cetearyl Alcohol	3	-	-	-	-	-	2.9	-	-	-	-
Citric Acid	1	0.9	-	1.5	-	-	-	1.7	-	-	-
Climbazole	7	-	-	-	2.9	-	-	-	-	-	-
Cocamide MEA	3	-	-	-	11.6	8.5	17.6	-	-	-	4.7
Cocamidopropyl Betaine	3	30.3	5.9	4.8	13.9	6.3	14.1	-	-	-	29.9
Cocamidopropyl Hydroxysultaine	3	-	-	-	-	-	-	14.7	-	-	-
Dimethicone	4	-	2.0	-	-	-	0.9	-	2.9	-	3.7
Dimethiconol	4	-	-	-	5.8	-	2.9	-	-	-	-
Dimethyl Lauramide/Myristamide	7	-	-	15.4	-	-	-	-	-	-	-
Disodium Cocoamphodiacetate	3	-	-	-	-	-	-	43.2	29.1	-	-
Disodium EDTA	1	1.4	-	-	-	1.2	-	-	-	-	-
Ethylene Brassylate	3	-	-	-	4.4	-	-	-	-	-	-
Glycerin	1	-	-	-	-	11.3	-	-	-	14.7	-
Glyceryl Caprylate/Caprate	3	-	-	-	-	-	-	-	-	5.2	-
Glycol Distearate	3	-	-	-	2.9	-	-	-	-	-	1.9
Glycol Stearate	3	-	-	-	-	-	2.9	-	8.7	-	-
Guar Hydroxypropyltrimonium Chloride	3	-	-	-	2.3	-	3.5	-	2.9	-	-
Helianthus Annuus Seed Oil	3	-	-	-	-	-	-	-	-	5.2	-
Hydrochloric Acid	1	-	-	-	-	-	-	-	-	-	3.0
Lanolin Wax	3	-	-	-	-	-	-	-	2.3	-	-
Lauryl Lactyl Lactate	3	-	-	2.6	-	-	-	-	-	5.2	-
Panthenol	1	-	-	-	-	-	0.6	-	-	-	-
PEG-150 Distearate	5	5.4	-	-	-	-	-	2.8	-	-	-
PEG-150 Pentaerythrityl Tetrastearate	6	-	-	-	-	1.4	-	-	-	-	-
PEG-80 Sorbitan Laurate	4	17.7	-	-	-	-	-	-	-	-	-
Phenoxyethanol	2	2.5	-	1.5	-	-	-	-	-	-	-
Polyquaternium-10	5	2.9	-	-	-	-	-	-	-	-	-
Polysorbate 20	4	-	-	-	-	8.5	-	-	-	-	-
PPG-12-Buteth-16	6	-	-	-	-	-	1.8	-	-	-	-
Propylene Glycol	2	-	-	-	-	-	-	-	-	-	3.7
Simmondsia Chinensis Seed Oil	3	-	-	-	-	-	-	-	-	5.2	-
Sodium Chloride	1	6.0	-	-	2.3	6.7	2.4	2.8	-	-	-
Sodium C12-18 Alkyl Sulfate	3	-	-	-	-	-	-	-	-	47.6	-
Sodium Hydroxide	1	-	1.2	-	-	-	-	-	-	-	-
Sodium Laureth Sulfate	3	-	20.6	21.2	48.7	51.3	45.3	-	48.8	-	48.6
Sodium Lauroamphoacetate	1	5.2	-	-	-	-	-	-	-	-	-
Sodium Lauryl Sulfate	2	-	61.3	47.7	-	-	-	-	-	-	-
Sodium Trideceth Sulfate	4	22.9	-	-	-	-	-	-	-	-	-
Percent Weight Considered		**95.4**	**94.9**	**94.9**	**97.5**	**95.1**	**95.0**	**94.9**	**94.7**	**99.0**	**95.5**
Overall Product Rank		**3**	**2**	**3**	**3**	**3**	**3**	**3**	**3**	**3**	**3**

Table S8 Ranking Results for Nine Facial Makeup Products

		Facial Makeup Product Name and Composition (Dry % w/w)								
INCI Name	**Rank**	**Foundation Stick**	**Concealer Stick**	**Creamy Stick Foundation**	**Cream-Powder Foundation**	**Liquid Foundation**	**Liquid Concealer**	**Powder Cream Concealer**	**Thin Liquid Foundation**	**Light Foundation**
Alcohol	2	-	-	-	-	-	-	-	7.0	-
Aluminum Hydroxide	1	-	-	-	-	0.8	-	-	-	-
Aluminum Starch Octenylsuccinate	2	10.0	-	-	-	-	-	-	-	-
Aluminum Stearate	2	-	-	-	-	-	-	-	-	2.5
Beeswax	3	-	6.7	3.0	-	-	-	-	-	-
Boron Nitride	4	-	-	5.0	-	-	-	-	-	-
Butylene Glycol	2	-	-	-	-	15.5	7.5	-	-	-
Butyloctyl Salicylate	3	-	-	-	-	-	-	-	-	5.9
C12-15 Alkyl Ethylhexanoate	3	21.5	-	-	-	-	-	-	-	-
C30-45 Alkyl Dimethicone	4	-	-	1.5	-	-	-	-	-	-
C30-45 Alkyl Methicone	4	-	-	-	-	-	-	3.4	-	-
Camelina Sativa Seed Oil	3	-	-	-	-	-	-	-	-	1.1
Caprylic/Capric Triglyceride	3	-	-	15.9	-	-	-	-	-	-
Cetyl Ethylhexanoate	3	-	-	5.0	-	-	-	-	-	-
Cyclohexasiloxane	6	-	-	-	-	-	-	-	41.2	-
Cyclopentasiloxane	7	-	-	-	-	-	-	-	1.7	38.9
Dimethicone	4	-	-	-	15.0	1.9	23.6	-	14.5	5.3
Dimethicone Crosspolymer	4	-	-	-	2.0	-	-	-	-	-
Dimethicone/PEG-10/15 Crosspolymer	4	-	-	-	-	-	-	-	-	3.2
Dimethicone/Vinyl Dimethicone Crosspolymer	4	-	-	-	-	-	-	-	0.8	-
Disteardimonium Hectorite	3	-	-	-	-	-	1.7	-	-	2.1
Ethyl Olivate	3	-	-	-	-	-	-	-	-	3.7
Ethylhexyl Methoxycinnamate (Octinoxate As Active Ingredient)	3	3.0	3.0	-	3.0	9.3	-	-	-	-
Ethylhexyl Palmitate	3	-	-	-	5.0	-	-	32.6	-	-
Euphorbia Cerifera (Candelilla) Wax	3	-	-	3.0	-	-	-	-	-	-
Glycerin	1	-	-	-	-	5.4	13.6	-	1.3	-
Glycol Stearate	3	-	-	-	-	4.2	-	-	-	-
HDI/Trimethylol Hexyllactone Crosspolymer	4	-	-	-	-	-	-	-	4.1	-
Iron Oxides	1	-	-	2.5	14.7	2.0	17.0	3.5	1.3	1.1
Isocetyl Stearate	5	-	-	-	-	15.8	-	-	-	-
Isododecane	8	-	-	-	-	-	-	-	1.9	-
Isohexadecane	9	-	-	-	-	-	-	-	1.2	-
Isopropyl Lanolate	7	-	5.8	-	-	-	-	-	-	-
Isopropyl Palmitate	3	-	-	-	9.4	-	-	-	-	-
Isostearyl Isostearate	5	-	-	24.2	-	-	-	-	-	-
Kaolin	1	-	-	-	2.0	-	-	-	-	-
Magnesium Aluminum Silicate	2	-	-	-	-	0.9	-	-	-	-
Mica	1	7.6	-	-	-	-	3.0	14.6	-	-
Nylon-12	5	5.0	6.0	10.0	2.0	-	-	-	-	-
Octyldodecyl Neopentanoate	3	-	-	-	-	1.9	-	-	-	-
Octyldodecyl Oleate	3	-	-	-	-	-	-	-	-	1.1
Olea Europaea (Olive) Leaf Extract	3	-	-	-	-	-	-	-	-	3.7
Ozokerite	5	-	9.3	-	3.0	-	-	-	-	-
PEG-10 Dimethicone	4	-	-	-	-	-	7.8	-	3.5	-
Phenoxyethanol	2	-	-	-	-	-	-	-	-	1.7
Phenyl Trimethicone	6	21.5	-	-	20.0	-	17.2	-	5.7	-
Polyethylene	5	5.0	2.3	-	6.0	-	-	-	-	-
Polymethyl Methacrylate	5	5.0	-	-	-	-	-	-	-	-
Polymethylsilsesquioxane	3	-	-	-	-	-	2.3	-	-	-
Polysorbate 60	2	-	-	-	-	4.5	-	-	-	-
PPG-2 Myristyl Ether Propionate	3	-	-	-	-	3.6	-	-	-	-
Propylene Carbonate	2	-	-	-	-	-	-	-	-	1.1
Propylene Glycol	2	-	-	-	-	-	-	-	-	6.3
Propylene Glycol Dicaprylate/Dicaprate	3	-	10.0	-	-	6.2	-	-	-	-
Silica	1	-	2.0	-	4.9	-	-	-	-	2.1
Sodium Chloride	1	-	-	-	-	-	2.2	-	-	-
Sorbitan Stearate	4	-	-	-	-	2.8	-	-	-	-
Squalane	5	-	24.6	-	-	-	-	-	-	-
Stearyl Dimethicone	4	5.0	-	-	-	-	-	-	-	-
Synthetic Wax	5	-	-	4.8	-	-	-	-	-	-
Talc	1	-	4.2	11.5	3.7	-	-	17.9	-	-
Tetrahexydecyl Ascorbate	3	-	-	0.5	-	-	-	-	-	-
Thymus Vulgaris Flower/Leaf/Stem Extract	3	-	-	-	-	-	-	-	-	1.1
Titanium Dioxide	1	12.2	20.0	8.1	-	19.7	-	19.6	10.4	2.1
Tribehenin	5	-	-	-	-	-	-	4.5	-	-
Vinyl Dimethicone Crosspolymer	4	-	-	-	-	-	-	-	-	2.1
Vinyl Dimethicone/Methicone Silsesquioxane Crosspolymer	4	-	-	-	2.0	-	-	-	-	-
Water	1	-	-	-	-	-	-	-	0.0	-
Zinc Oxide	7	-	2.2	-	2.2	-	-	-	-	10.1
Percent Weight Considered		**95.8**	**96.0**	**94.9**	**94.8**	**94.5**	**95.9**	**96.0**	**94.7**	**94.8**
Overall Product Rank		**3**	**4**	**3**	**3**	**2**	**3**	**2**	**4**	**5**