SUPPORTING INFORMATION

Applying Green Chemistry to Raw Material Selection and Product Formulation at The Estée Lauder Companies

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Table S1. Human Health Scoring Rubric

Endpoint description/Source	Score	Score assignment rubric
Acute toxicity: Assesses the inherent lethality hazard via ingestion, inhalation, and dermal absorption exposure routes. The primary data sources are the GHS classification for acute toxicity and the Canada DSL HH priorities classification. If data are present in both the GHS and DSL, the lower (more conservative) score is taken	1	Acute toxicity 1 GHS classification OR DSL HH priorities label is “high” or “post 2006”
	2	Acute toxicity 2 GHS classification OR DSL HH priorities label is “moderate”
	3	Acute toxicity 3 GHS classification
	4	Acute toxicity 4 GHS classification OR DSL HH priorities label is “low”
	5	No acute toxicity GHS classifications AND no DSL HH priorities label is present
Ocular toxicity: Assesses the inherent hazard to cause eye damage and/or irritation. The primary data sources are the GHS classifications for eye irritation and eye damage	1	Eye damage GHS classification
	3	Eye irritation GHS classification
	5	No eye damage or eye irritation GHS classifications present
Dermal toxicity: Assesses the inherent hazard to cause dermal corrosion, irritation, and/or sensitization. The primary data sources are the GHS classifications for skin corrosion, skin irritation, skin mild irritation, and skin sensitization	1	Skin sensitization 1A OR any skin corrosion GHS classification
	2	Any skin irritation GHS classification
	3	Skin sensitization 1B or skin sensitization 1 GHS classification
	4	Skin mild irritation GHS classification
	5	No skin corrosion, skin irritation, skin mild irritation, or skin sensitization GHS classifications present

DSL, Domestic Substance List; GHS, Globally Harmonized System of Classification and Labelling of Chemicals; HH, human health.

Table S2. Ecosystem Health Scoring Protocol

Endpoint description/Source	Score	Score assignment rubric
Bioaccumulation: Assesses the propensity to bioaccumulate up the food chain when free in the environment. The primary data source is the Canada DSL bioaccumulation classification. The secondary data source is the component's feedstock sourcing data, as provided by the raw material supplier to ELC	1	DSL bioaccumulation label is "yes"
	2	DSL bioaccumulation label is blank
	3	DSL bioaccumulation label is "uncertain"
	4	Component is not listed in the DSL, and feedstock source is wholly biological or mineral
	5	DSL bioaccumulation label is "no"
Persistence: Assesses the propensity to persist (i.e., not break down or biodegrade) when free in the environment. The primary data source is the Canada DSL persistence classification. The secondary data source is the component's feedstock sourcing data, as provided by the raw material supplier to ELC	1	DSL persistence label is "yes"
	2	DSL persistence label is blank
	3	DSL persistence label is "uncertain"
	4	Component is not listed in the DSL, and feedstock source is wholly biological or mineral
	5	DSL persistence label is "no"
Aquatic toxicity: Assesses the inherent hazard in the aquatic environment, both acutely and chronically. The primary data sources are the GHS classifications for aquatic acute toxicity and aquatic chronic toxicity, along with the DSL inherently toxic to aquatic organisms classification. The more conservative score is taken. If no information is present in the DSL database, it is scored according to the GHS	1	Aquatic acute 1 or aquatic chronic 1 GHS classification OR DSL inherently toxic to aquatic organisms label is "yes"
	2	Aquatic chronic 2 GHS classification OR DSL inherently toxic to aquatic organisms label is blank
	3	Aquatic chronic 3 GHS classification OR DSL inherently toxic to aquatic organisms label is "uncertain"
	4	Aquatic chronic 4 GHS classification
	5	No aquatic acute or aquatic chronic GHS classifications AND DSL inherently toxic to aquatic organisms label is "no"

DSL, Domestic Substance List; ELC, Estée Lauder Companies; GHS, Globally Harmonized System of Classification and Labelling of Chemicals.

Table S3. Environment Scoring Protocol

Endpoint description/Source	Score	Score assignment rubric
Feedstock sourcing: Assesses for ingredient's environmental impact of sourcing, degree of supply chain transparency, and whether it has a third-party sustainability certification. All data are obtained from ELC suppliers. Three independent submetrics are added to score this metric: - Ingredient composition: Assesses for % of petroleum-derived content - Ingredient geography: Assesses for sourcing transparency - Certifications: Assesses for any RSPO or organic certifications	1	Ingredient source is wholly of petroleum origin
	2	Ingredient source is partially of petroleum origin and partially of biological or mineral origin
	3	Ingredient source is wholly of biological or mineral origin
	+1 Point	All ingredient components have an associated country of origin
	+1 Point	Ingredient is RSPO certified (e.g., mass balance) or certified organic (USDA or COSMOS)
GHG emissions: Assesses ingredient's GHG impact. Calculated by averaging 2 independent submetrics: - GHG supplier emissions: Scopes 1 & 2 emissions effect per kilogram of product, as provided by ELC suppliers - GHG modelled emissions: Scopes 1, 2 & 3 emissions effect of each ingredient component, as obtained from the ecoinvent 3 database, per the component chemical classification. The ingredient GHG modelled emissions score is calculated via the mass-weighted average of its components' scores	1	GHG supplier value/modelled emissions factor is >1000
	2	GHG supplier emissions: No GHG emissions information is provided by the supplier
	$5 - [\log_{10}(x) + 1]$	GHG supplier value/modelled emissions factor (x) is >0.1 but <1000
	5	GHG supplier value/modelled emissions factor is <0.1

COSMOS, COSMetic Organic and Natural Standard; ELC, Estée Lauder Companies; GHG, greenhouse gas; RSPO, Roundtable on Sustainable Palm Oil; USDA, US Department of Agriculture.

Table S4. Default Scoring Proxies

Default type	Acute toxicity	Ocular toxicity	Dermal toxicity	Bioaccumulation	Persistence	Aquatic toxicity
Biological	5	3	3	4	4	5
Mineral	3	3	3	4	4	3
Fluoro compound	2	2	2	3	1	2
Colorant	5	3	3	3	2	2
Polymer	4	3	3	5	1	4
Siloxane/Silicone	4	2	2	5	1	4
Natural metabolite	4	4	4	5	5	4
Petroleum	2	2	2	3	3	2
Unknown	3	3	3	3	3	3

Table S5. Certainty Score Assignment

Endpoint	Score	Score assignment
All HH and ECO endpoints	2	From default data value
	3	From proxy data value
	5	From GHS or DSL data
ENV feedstock sourcing	3	All raw materials
ENV greenhouse gas emissions	2	From default data value
	4	From individual chemical

DSL, Domestic Substance List; ECO, ecosystem health; ENV, environment; GHS, Globally Harmonized System of Classification and Labelling of Chemicals; HH, human health.

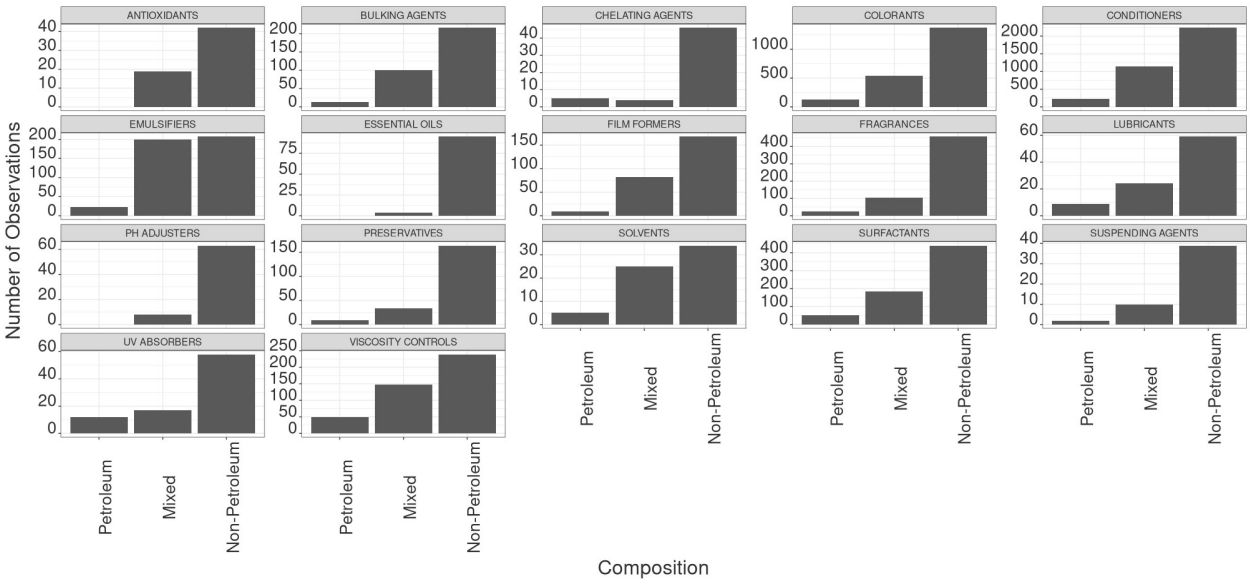
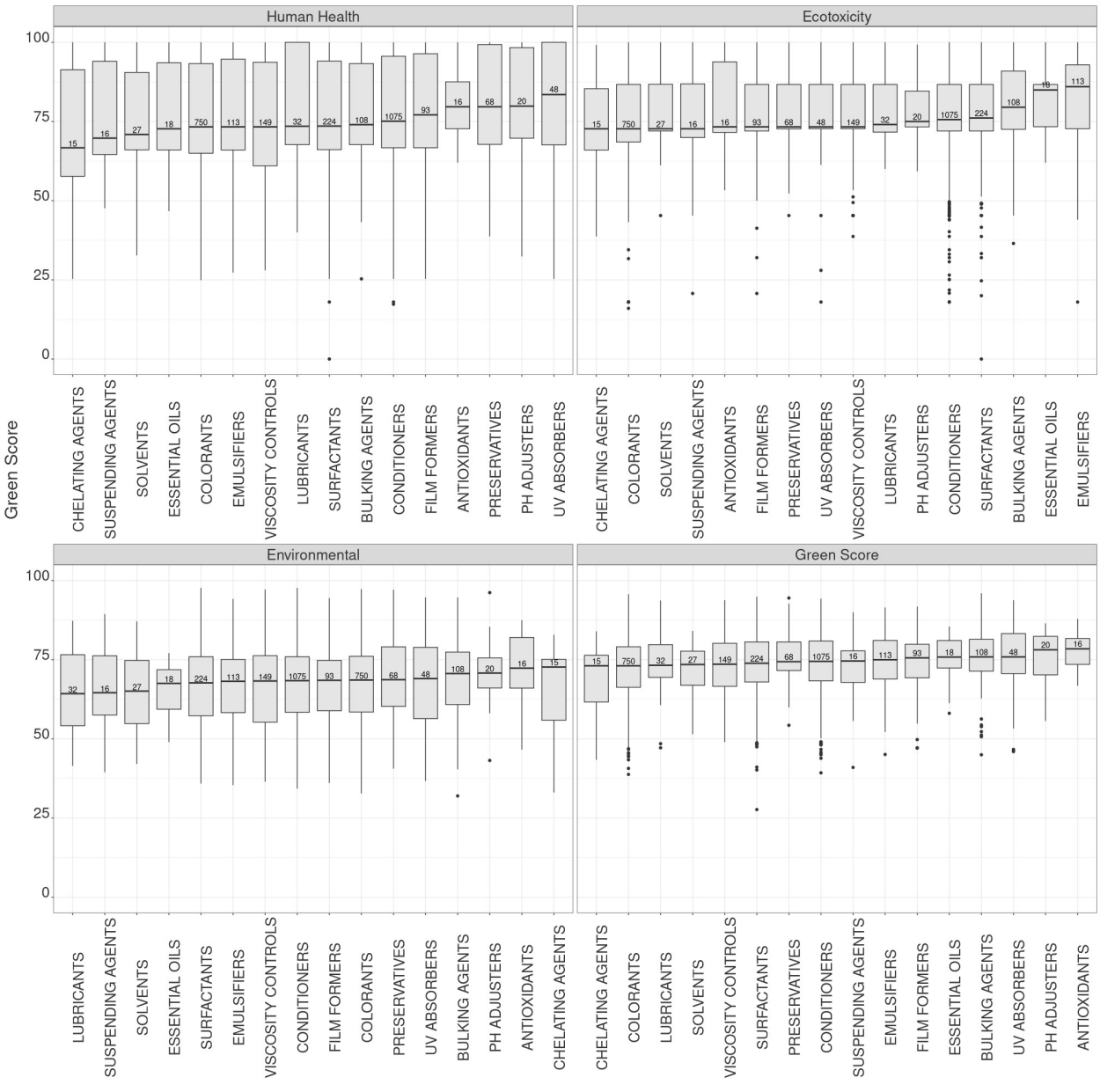
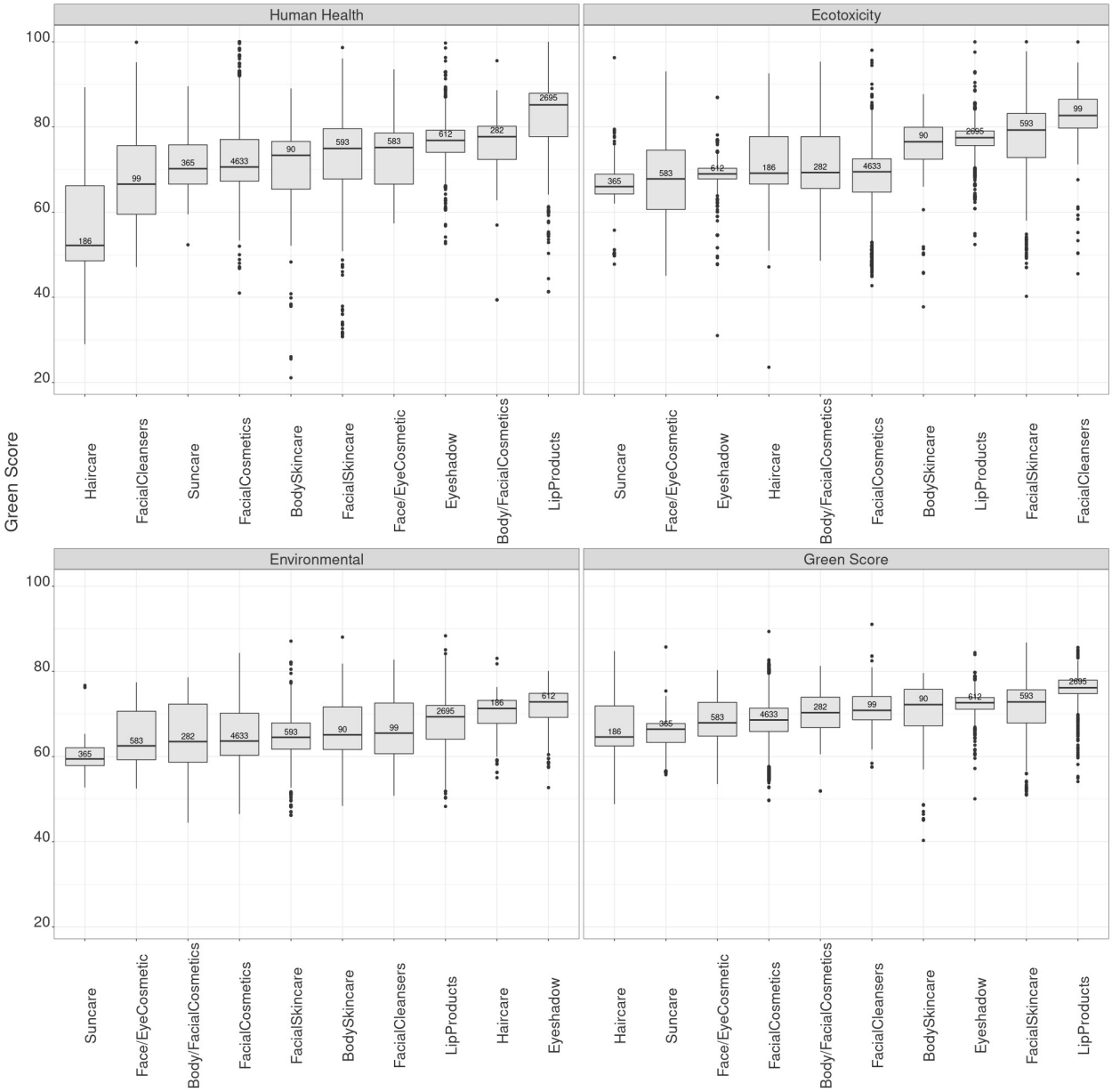


Figure S1. Number of pure petroleum, mixed, or non-petroleum chemicals for each functional class.


Human Health
Ecotoxicity
Environmental
Green Score
Green Score
100
75
50
25
0
CHELATING AGENTS
SUSPENDING AGENTS
SOLVENTS
ESSENTIAL OILS
COLORANTS
EMULSIFIERS
VISCOSITY CONTROLS
LUBRICANTS
SURFACTANTS
BULKING AGENTS
CONDITIONERS
FILM FORMERS
ANTIOXIDANTS
PRESERVATIVES
PH ADJUSTERS
UV ABSORBERS


Human Health
Ecotoxicity
Environmental
Green Score
Green Score
100
80
60
40
20
Haircare
FacialCleansers
Suncare
FacialCosmetics
BodySkincare
FacialSkincare
Face/EyeCosmetic
Eyeshadow
Body/FacialCosmetics
LipProducts
Suncare
Face/EyeCosmetic
Eyeshadow
Haircare
Body/FacialCosmetics
FacialCosmetics
BodySkincare
LipProducts
FacialSkincare
FacialCleansers
Suncare
Face/EyeCosmetic
Body/FacialCosmetics
FacialCosmetics
FacialSkincare
BodySkincare
FacialCleansers
LipProducts
Haircare
Eyeshadow
Haircare
Suncare
Face/EyeCosmetic
FacialCosmetics
Body/FacialCosmetics
FacialCleansers
BodySkincare
Eyeshadow
FacialSkincare
LipProducts

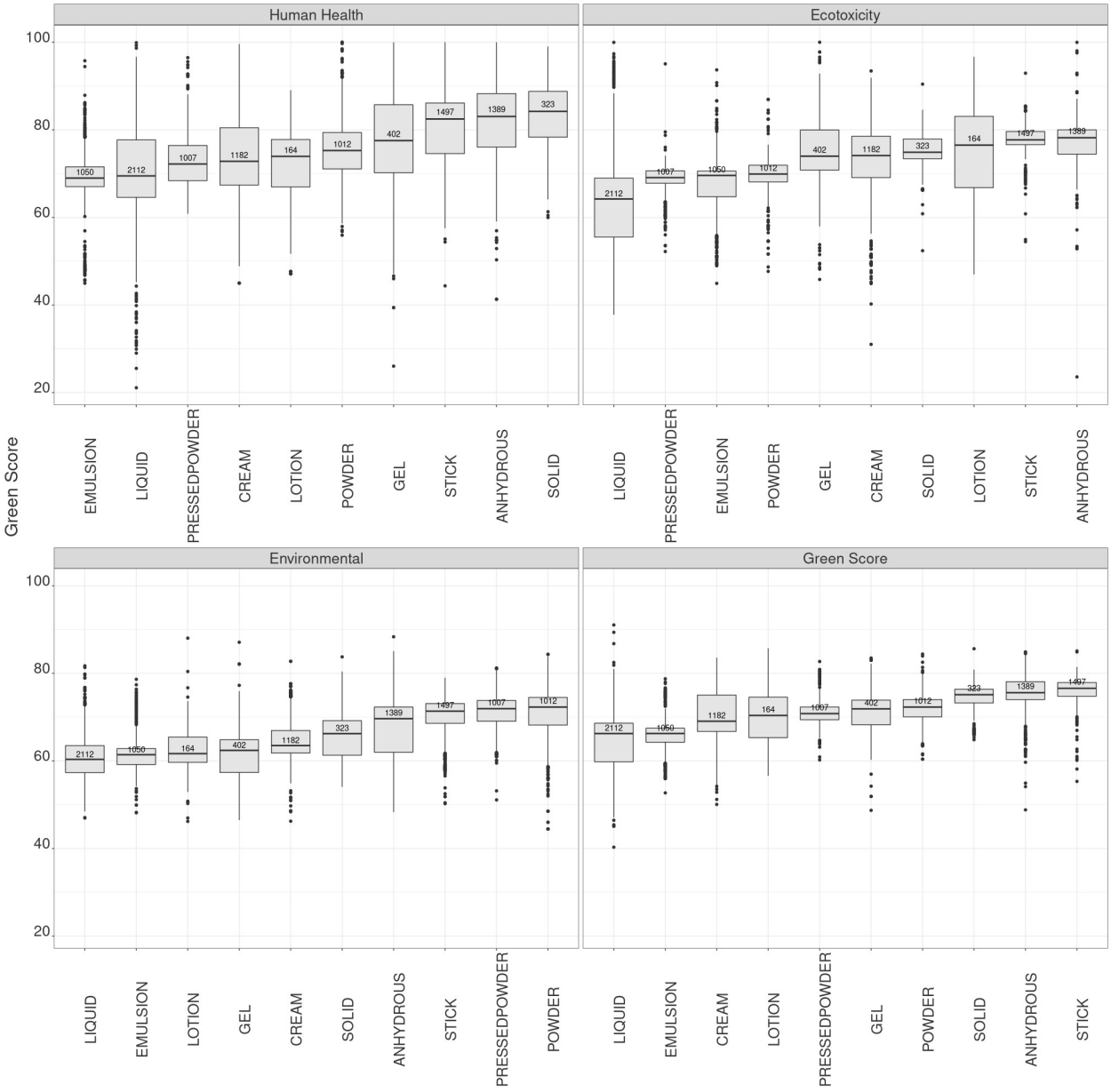


Figure S2. Distribution of Green Scores **(A)** at the raw material level by functional class, **(B)** by product category, and **(C)** by product form. Number of observations within each group is listed above the median.

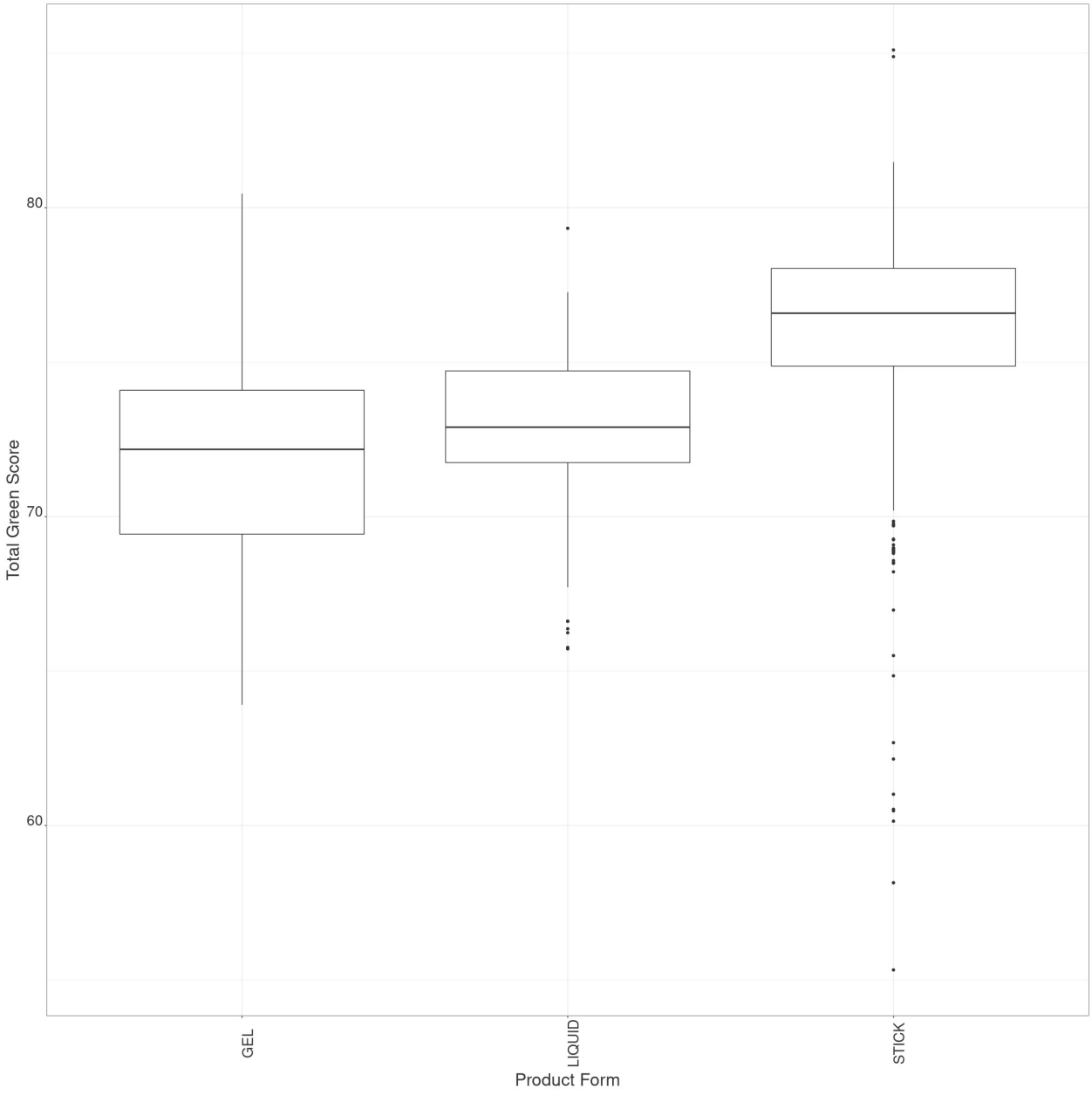
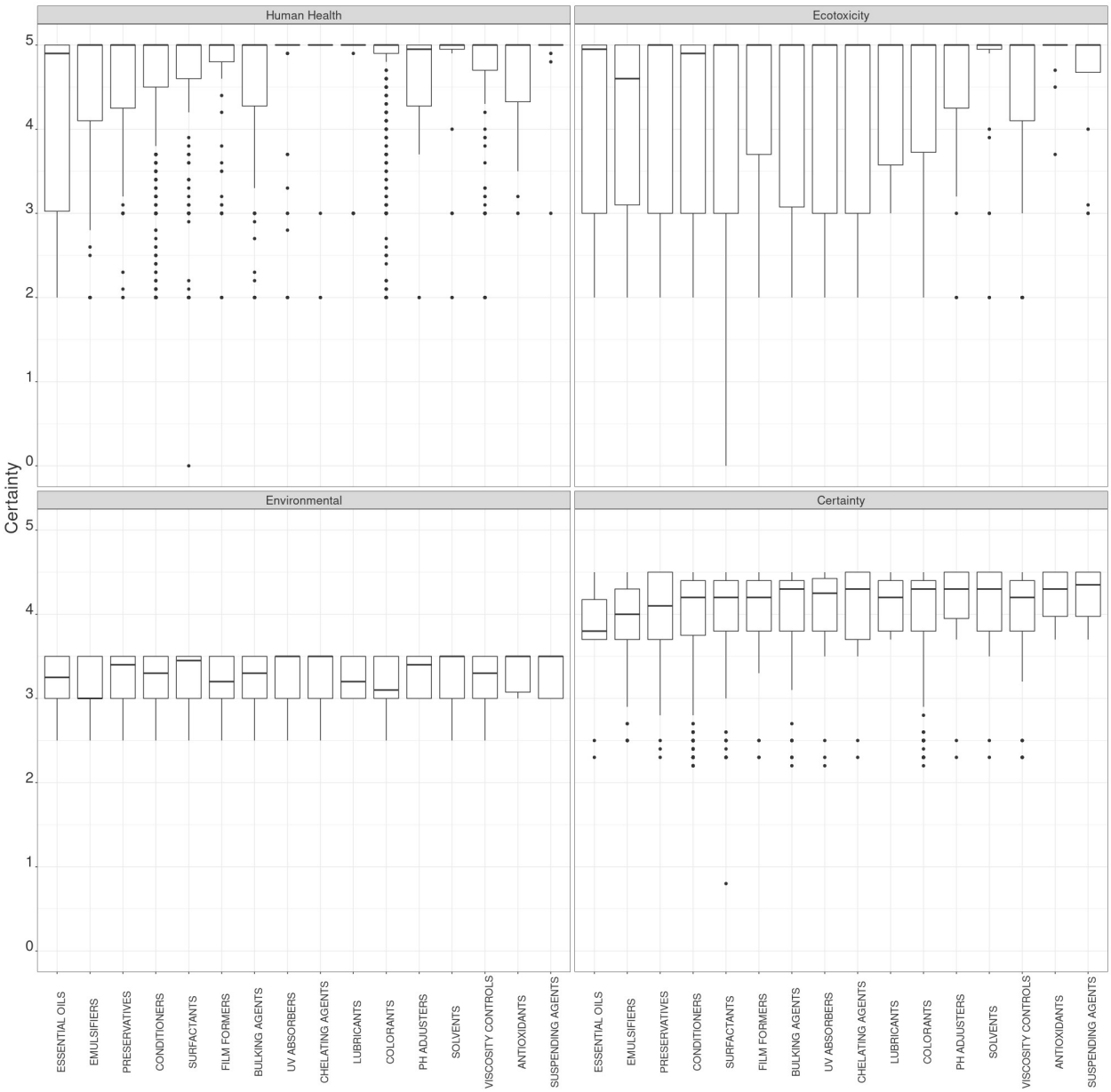
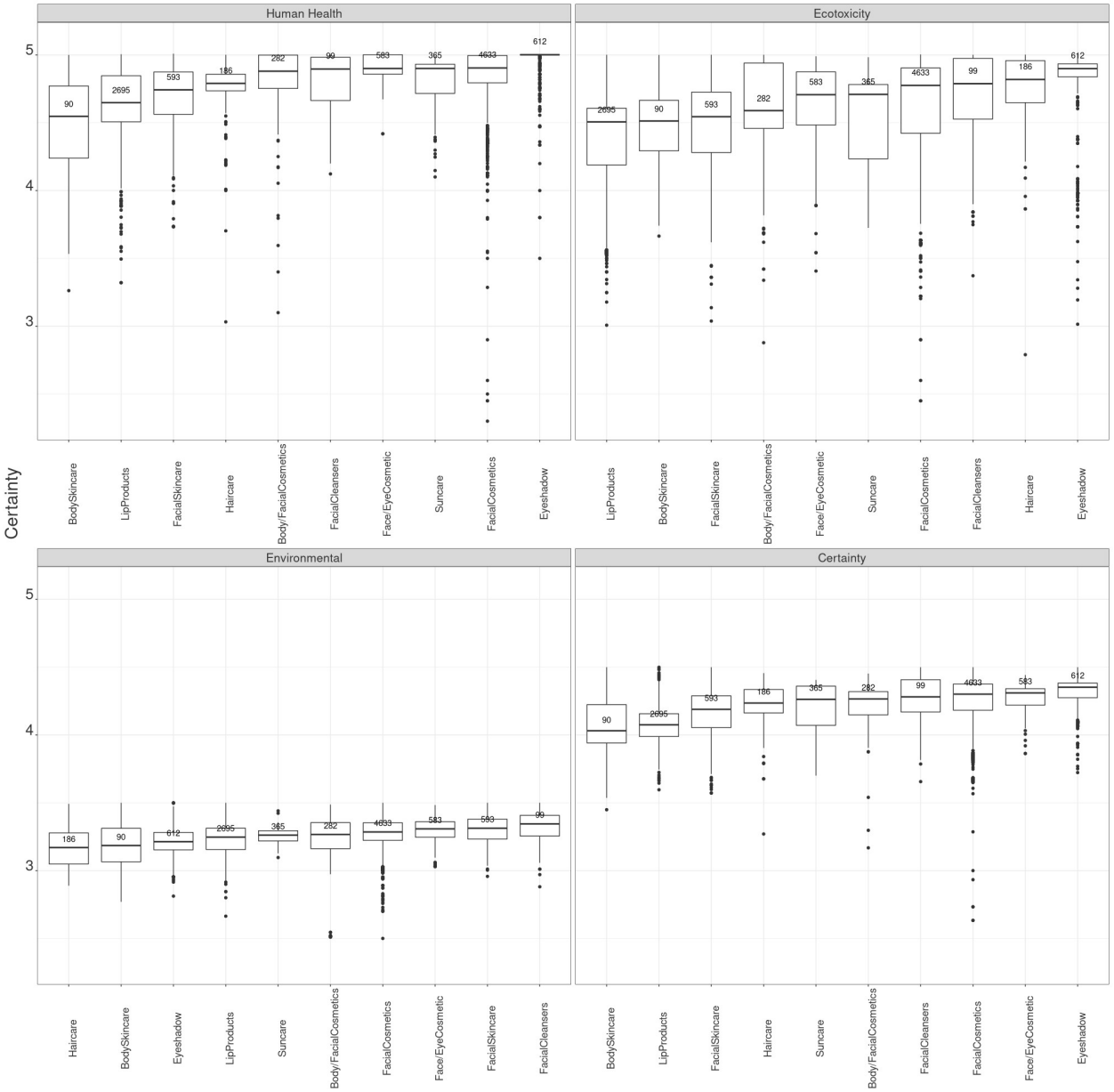


Figure S3. Distribution of Green Scores for the product category of lip care by product form.


Human Health
Ecotoxicity
Environmental
Certainty
Certainty
0
1
2
3
4
5
ESSENTIAL OILS
EMULSIFIERS
PRESERVATIVES
CONDITIONERS
SURFACTANTS
FILM FORMERS
BULKING AGENTS
UV ABSORBERS
CHELATING AGENTS
LUBRICANTS
COLORANTS
PH ADJUSTERS
SOLVENTS
VISCOSITY CONTROLS
ANTIOXIDANTS
SUSPENDING AGENTS


Human Health
Ecotoxicity
Environmental
Certainty
Certainty
5
4
3
90
2695
593
186
282
99
583
365
4633
612
BodySkincare
LipProducts
FacialSkincare
Haircare
Body/FacialCosmetics
FacialCleansers
Face/EyeCosmetic
Suncare
FacialCosmetics
Eyeshadow

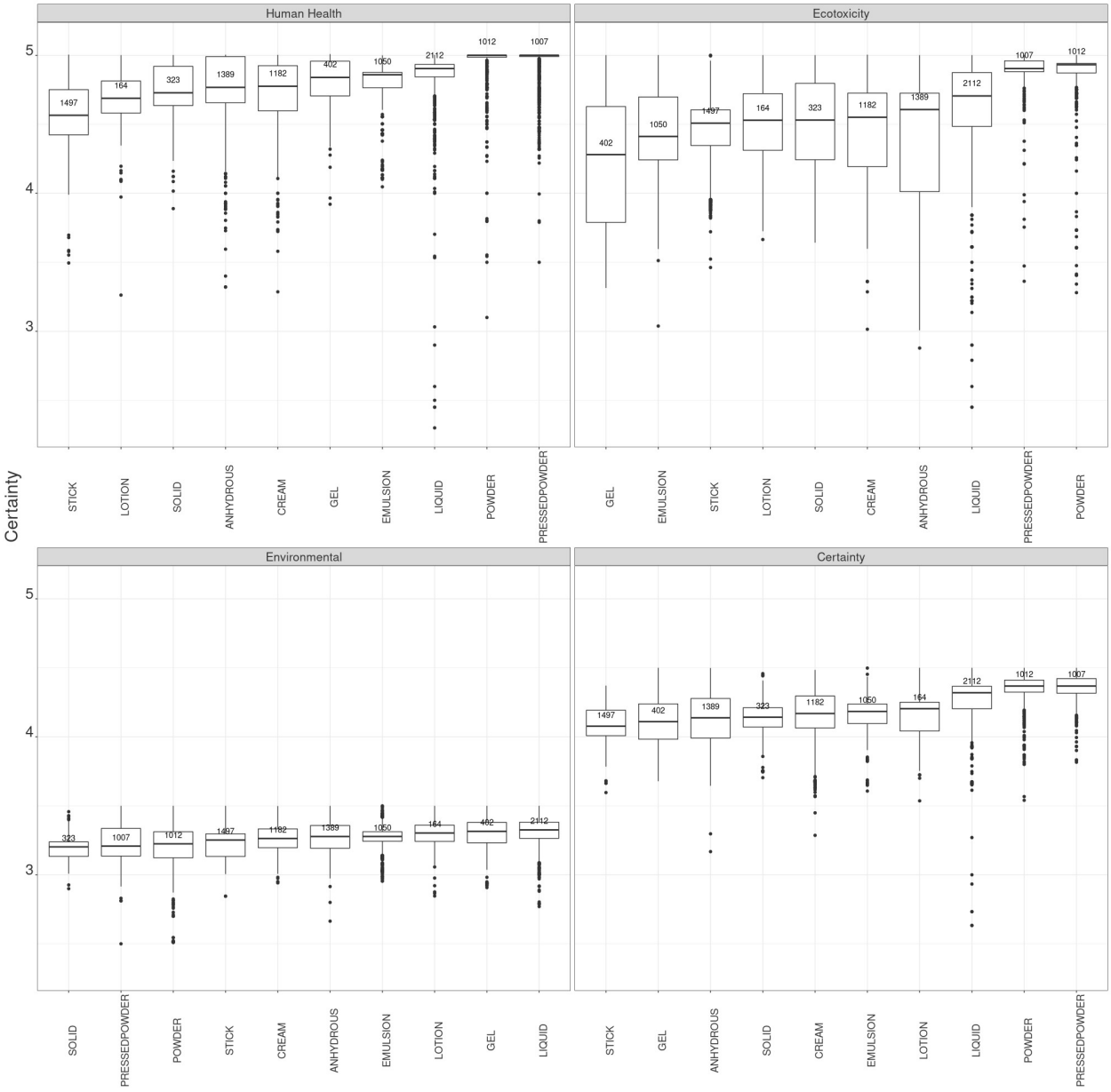


Figure S4. Certainty scores by **(A)** functional class of raw materials, **(B)** product category, and **(C)** product form. Number of observations within each group is listed above the median.