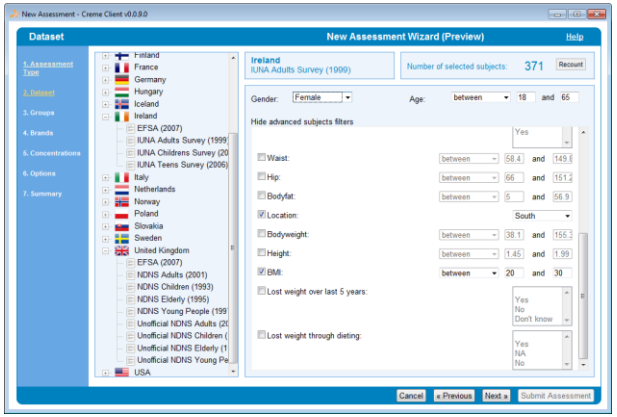
Expert Models for Decision Makers ™

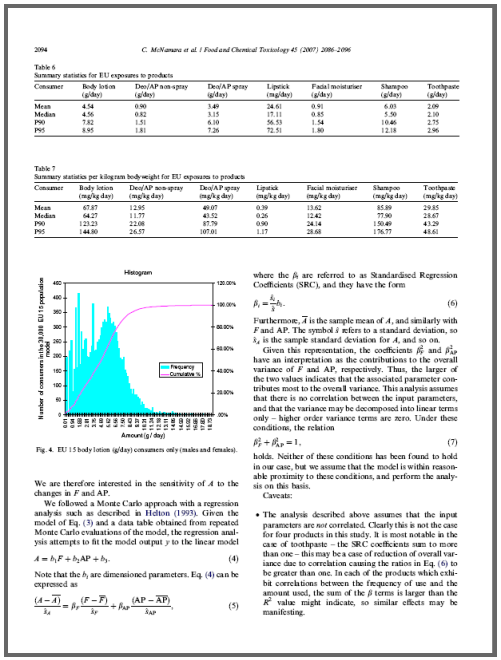
The Truth is Out There:

Combining private data sets to assess human health risks

Cronan McNamara
Co-founder & CEO, Creme Global
Founder, Predict Conference
Chair, Irish Software Association

Creme Global - Services





2094 C. McNamara et al. / Food and Chemical Toxicology 45 (2007) 2086–2096

Table 6
Summary statistics for EU exposures to products

Consumer	Body lotion (g/day)	Deo/AP non-spray (g/day)	Deo/AP spray (g/day)	Lipstick (mg/day)	Facial moisturiser (g/day)	Shampoo (g/day)	Toothpaste (g/day)
Mean	4.54	0.90	3.49	24.61	0.91	6.03	2.09
Median	4.56	0.82	3.15	17.11	0.85	5.50	2.10
P90	7.82	1.51	6.10	56.53	1.54	10.46	2.75
P95	8.95	1.81	7.26	72.51	1.80	12.18	2.96

Table 7
Summary statistics per kilogram bodyweight for EU exposures to products

Consumer	Body lotion (mg/kg day)	Deo/AP non-spray (mg/kg day)	Deo/AP spray (mg/kg day)	Lipstick (mg/kg day)	Facial moisturiser (mg/kg day)	Shampoo (mg/kg day)	Toothpaste (mg/kg day)
Mean	67.87	12.95	49.07	0.39	13.62	85.89	29.85
Median	64.27	11.77	43.52	0.26	12.42	77.90	28.67
P90	123.23	22.08	87.79	0.90	24.14	150.49	43.29
P95	144.80	26.57	107.01	1.17	28.68	176.77	48.61

Histogram

Fig. 4. EU 1.5 body lotion (g/day) consumers only (males and females).

We are therefore interested in the sensitivity of A to the changes in F and AP.

We followed a Monte Carlo approach with a regression analysis such as described in Helton (1993). Given the model of Eq. (3) and a data table obtained from repeated Monte Carlo evaluations of the model, the regression analysis attempts to fit the model output y to the linear model

$$A = b_1 F + b_2 \mathrm{AP} + b_3. \quad (4)$$

Note that the b_i are dimensioned parameters. Eq. (4) can be expressed as

$$\frac{(A-\overline{A})}{\lambda_A} = \beta_F \frac{(F-\overline{F})}{\lambda_F} + \beta_{\mathrm{AP}} \frac{(\mathrm{AP}-\overline{\mathrm{AP}})}{\lambda_{\mathrm{AP}}}. \quad (5)$$

where the β_i are referred to as Standardised Regression Coefficients (SRC), and they have the form

$$\beta_i = \frac{\lambda_i}{\lambda_y} b_i. \quad (6)$$

Furthermore, $\overline{A}$ is the sample mean of A, and similarly with F and AP. The symbol λ refers to a standard deviation, so λ_A is the sample standard deviation for A, and so on.

Given this representation, the coefficients β_F^2 and β_{AP}^2 have an interpretation as the contributions to the overall variance of F and AP, respectively. Thus, the larger of the two values indicates that the associated parameter contributes most to the overall variance. This analysis assumes that there is no correlation between the input parameters, and that the variance may be decomposed into linear terms only – higher order variance terms are zero. Under these conditions, the relation

$$\beta_F^2 + \beta_{A,P}^2 = 1. \quad (7)$$

holds. Neither of these conditions has been found to hold in our case, but we assume that the model is within reasonable proximity to these conditions, and perform the analysis on this basis.

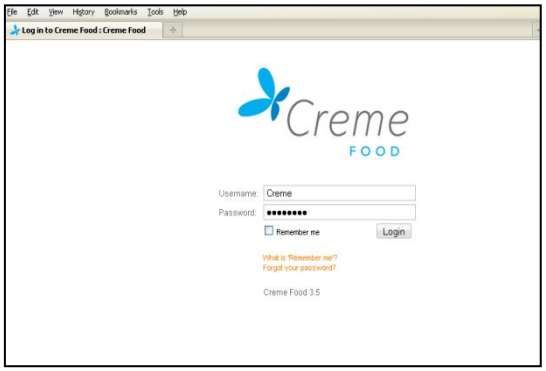
Caveats:

- The analysis described above assumes that the input parameters are *not* correlated. Clearly this is not the case for four products in this study. It is most notable in the case of toothpaste – the SRC coefficients sum to more than one – this may be a case of reduction of overall variance due to correlation causing the ratios in Eq. (6) to be greater than one. In each of the products which exhibit correlations between the frequency of use and the amount used, the sum of the β terms is larger than the R^2 value might indicate, so similar effects may be manifesting.

High Performance Cloud Software

Technical Services & Projects

Data Collection & Modeling

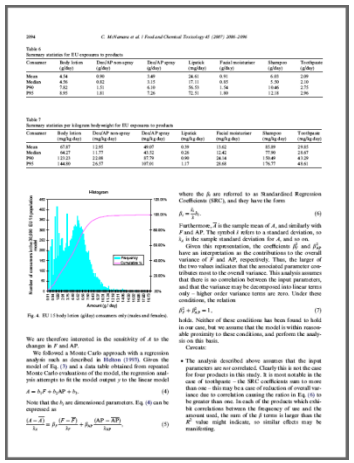


Creme GLOBAL

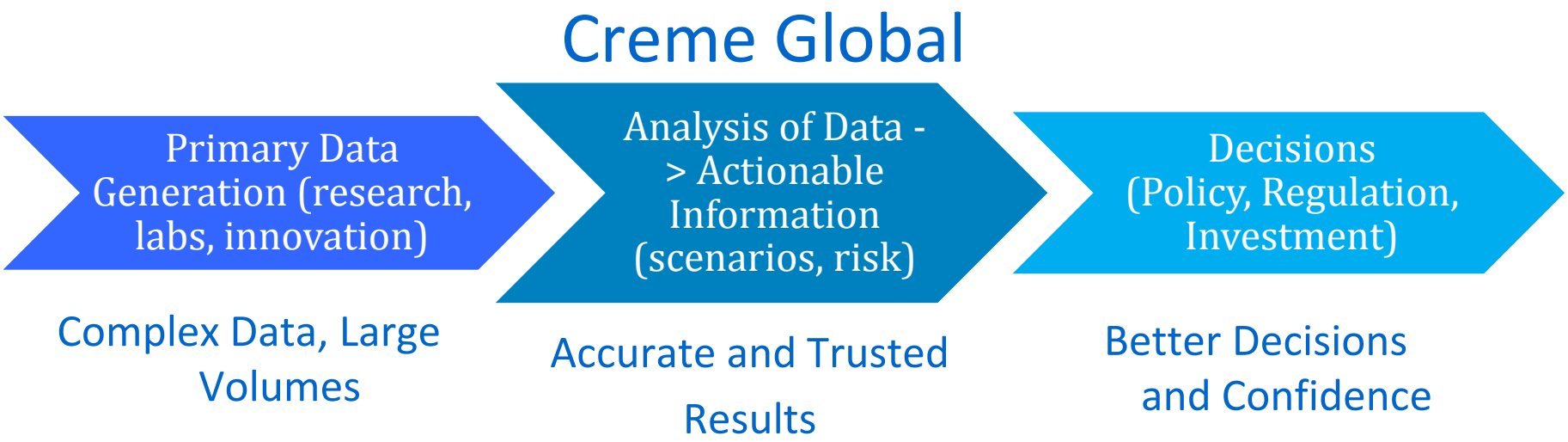
Cloud Software

Technical Services

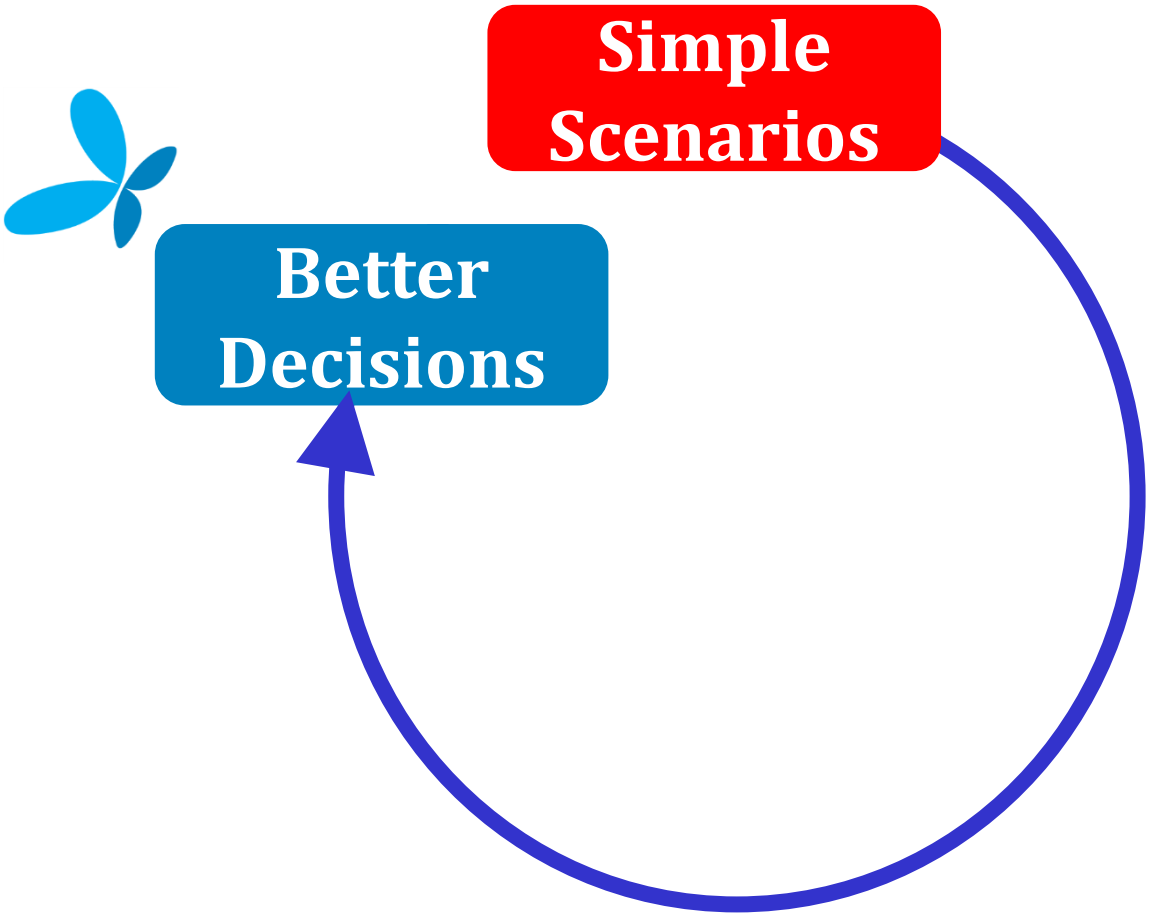
Data Curation



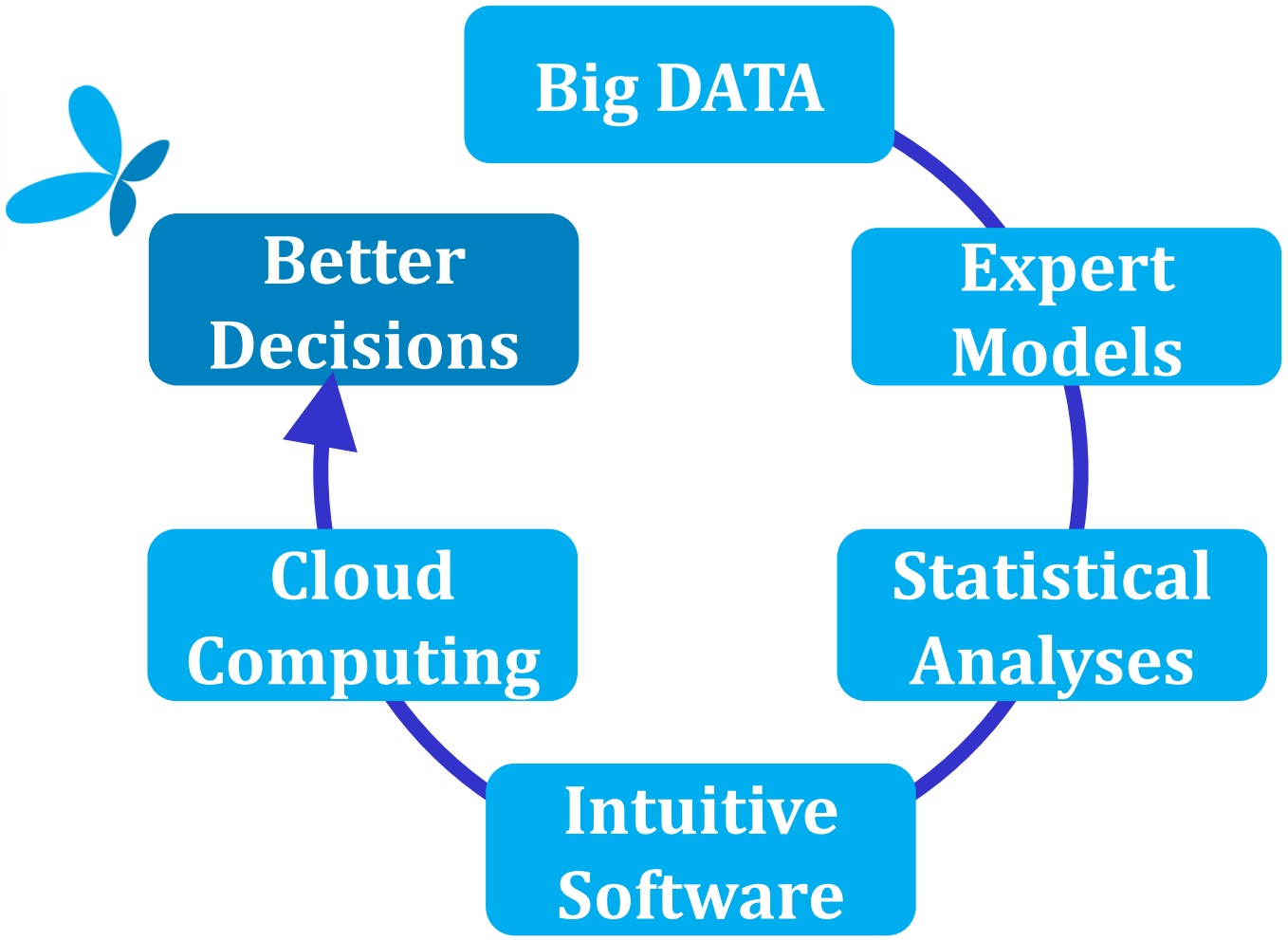
Value Chain


Creme Global
Primary Data Generation (research, labs, innovation)
Analysis of Data -> Actionable Information (scenarios, risk)
Decisions (Policy, Regulation, Investment)
Complex Data, Large Volumes
Accurate and Trusted Results
Better Decisions and Confidence

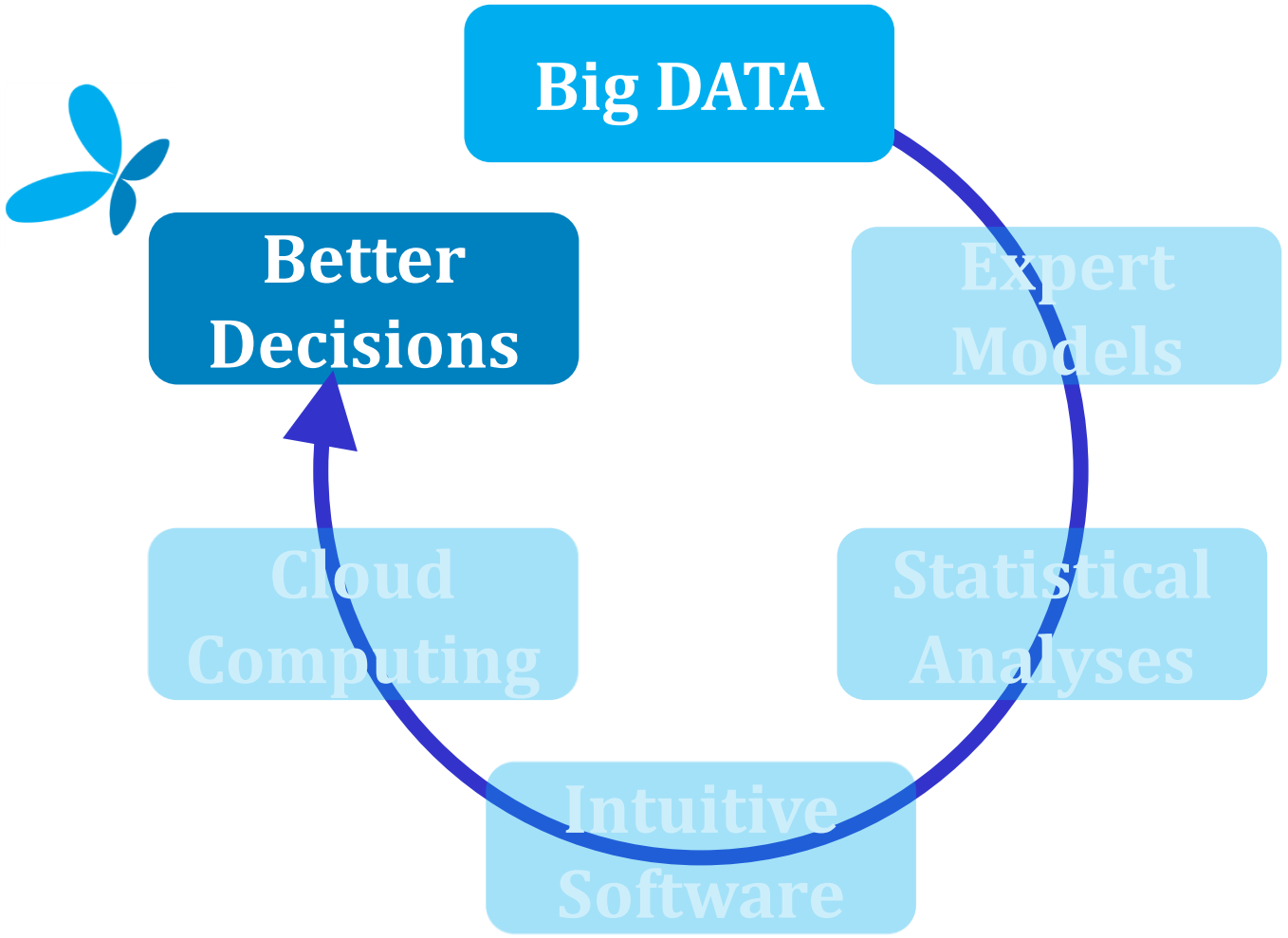
Revolution in Decision Making



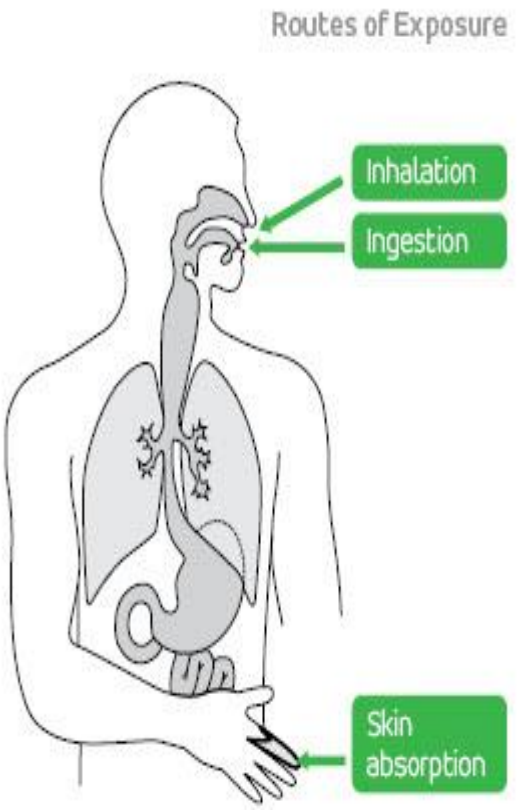
Revolution in Decision Making



Revolution in Decision Making



Predictive Intake Modelling



- Foods
- Nutrients
- Cosmetics
- Consumer products
- Chemicals
- Bacteria

Two Questions

How are consumers exposed to substances from food packaging?

How much do fragrances get on to our skin and into our bodies?

How are consumers exposed to substances from food packaging?

FOOD PACKAGING

Creme GLOBAL

Project Goal:

Develop a robust database, model and software to assess consumer exposure in Europe

Linking Foods to Substances

Food Consumption Data

Food Categories

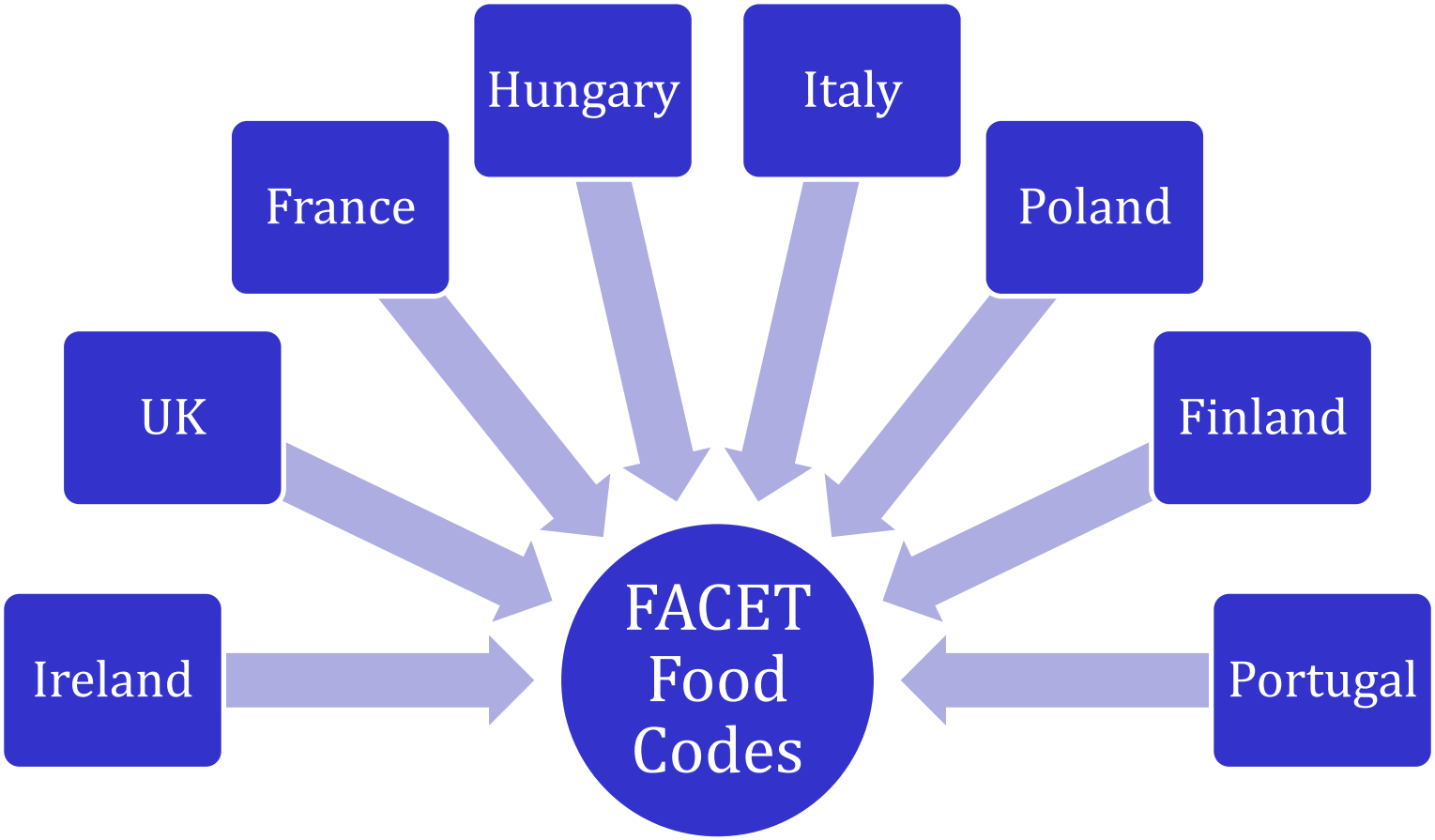
Packaging Type

Structures

Materials

Chemical Substances

Food Intakes - Dietary Surveys



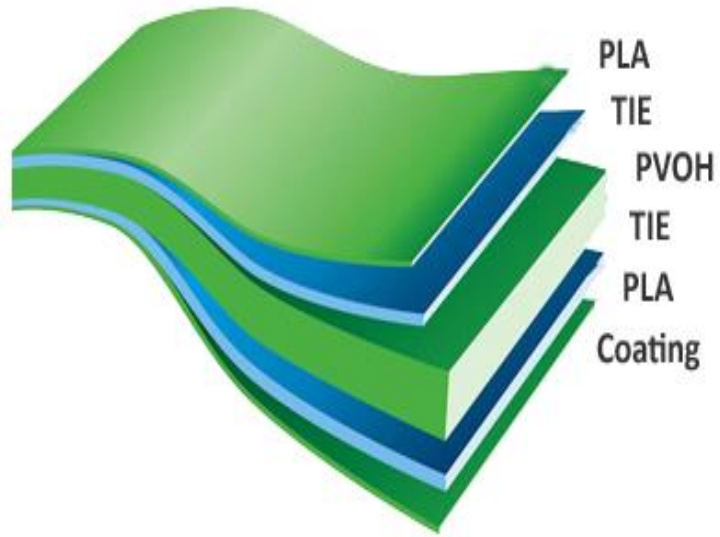
Packaging Type

Market Survey Data

Inputs

- Packaging type by food category
- Pack size
- Contact areas
- Market shares

Structures and Materials



- Industry source
- Layer materials and thicknesses
- Time/temperature

Chemical Substances

- Raw material composition
- Chemical concentrations
- Probability of occurrence

Migration Model

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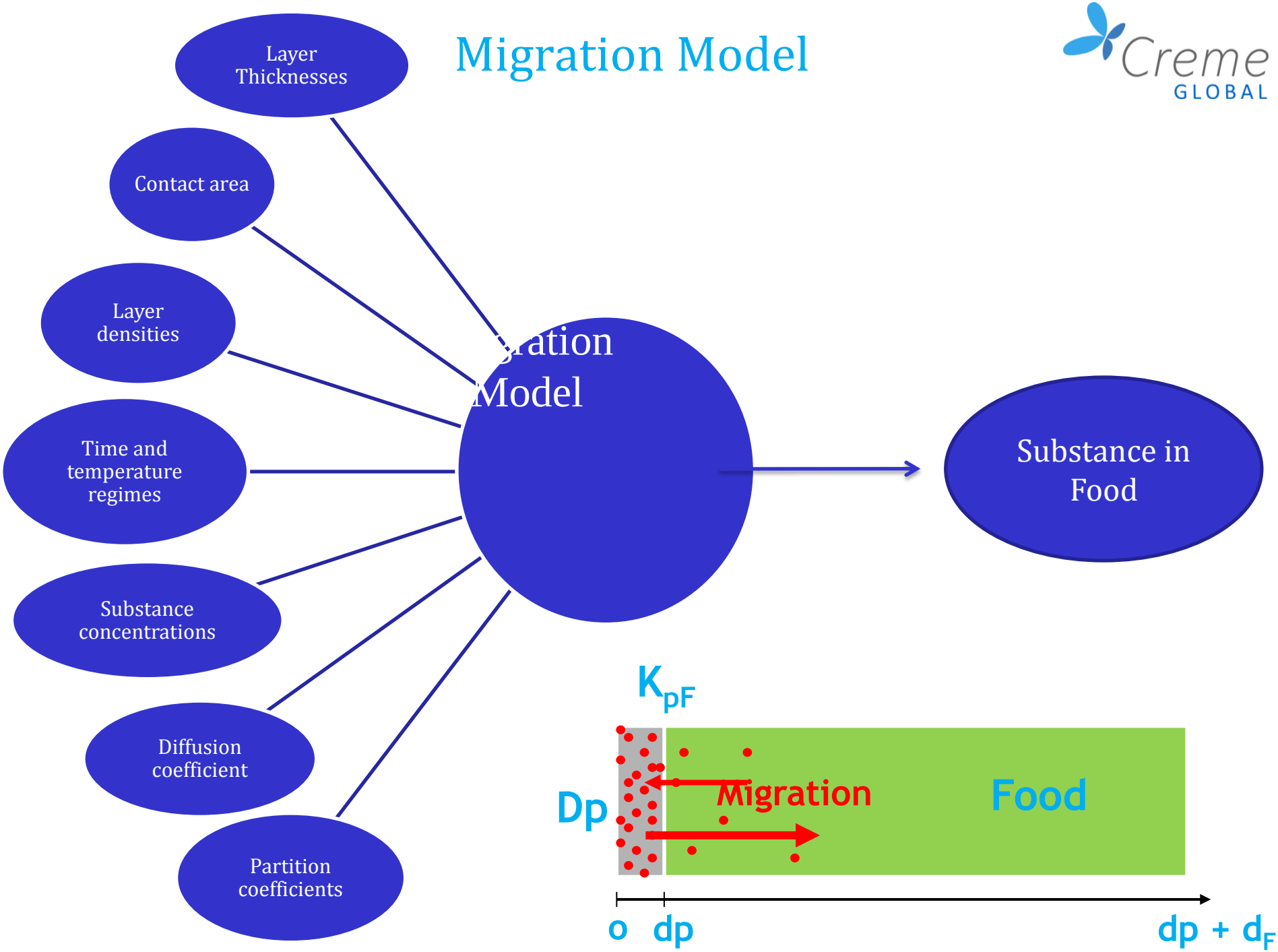


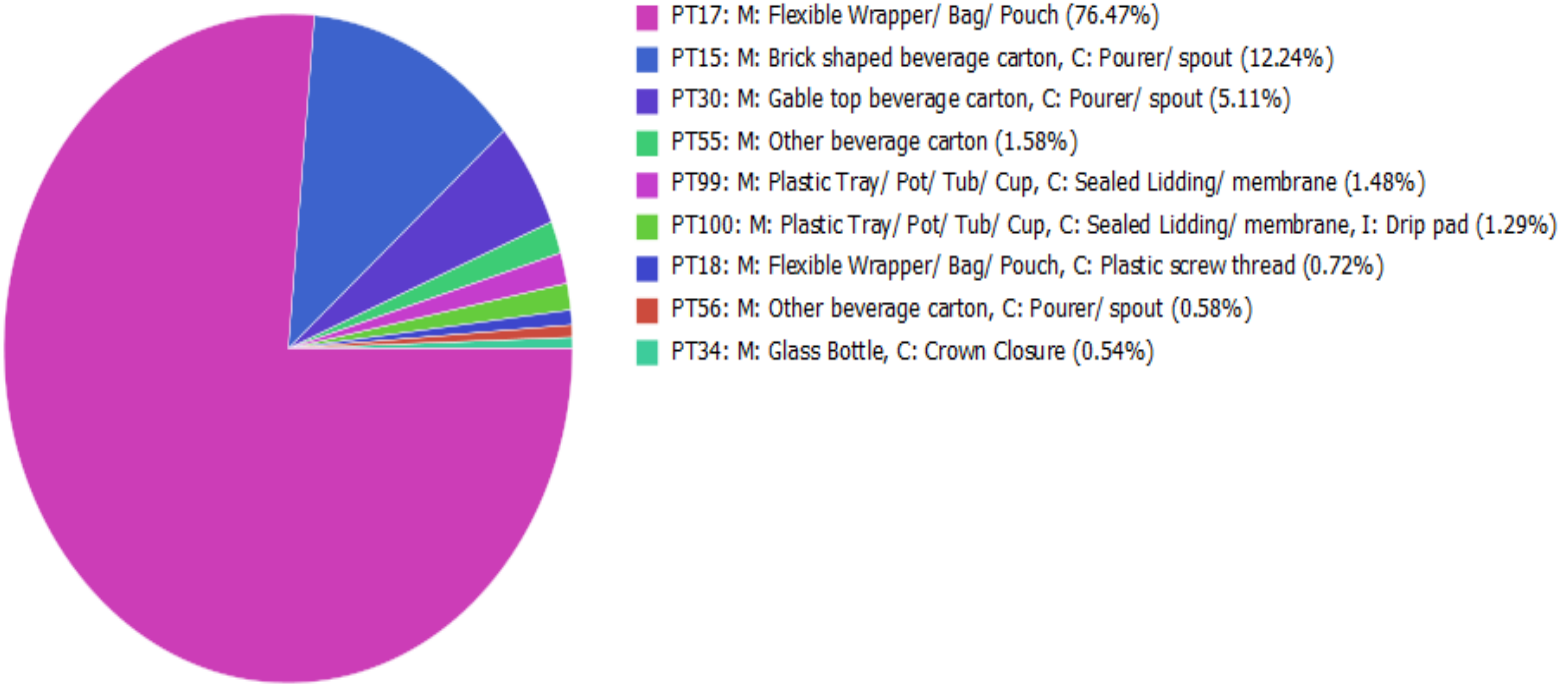
FACET

File Changes New Help

By Food Category | By Pack Type

Home | Assessments | FACET Data | My Data | Results - Irganox...

All - Per unit body weight - Total Population - Mean



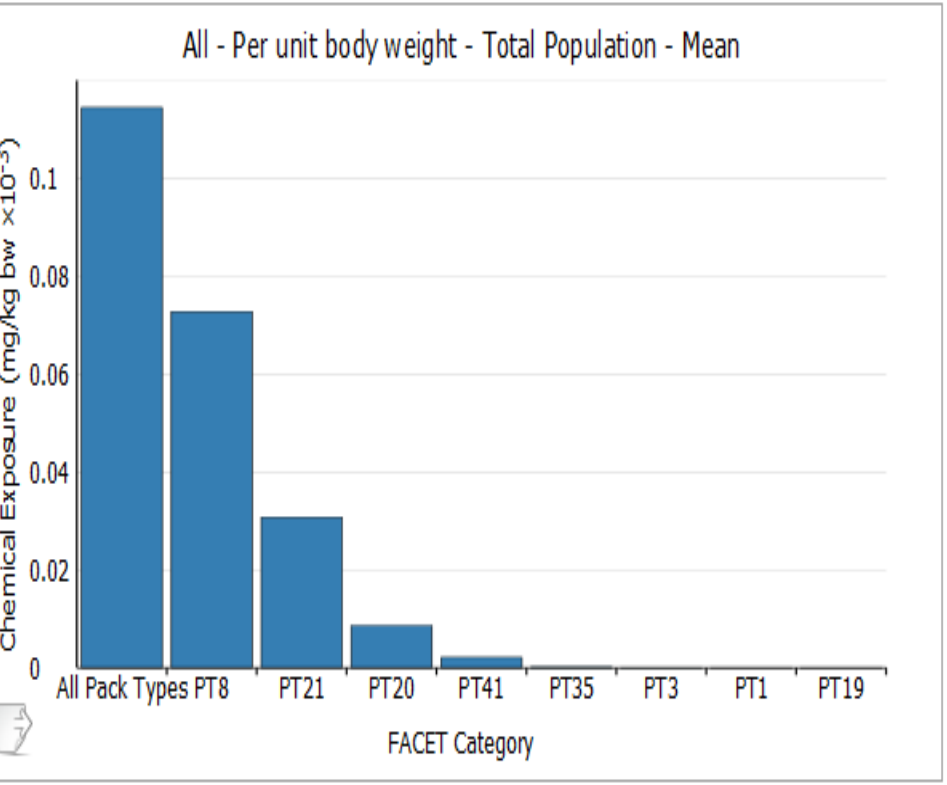
Pack Type Description	Intake Type	Consumer T...	FACET Category Co...	FACET Category Na...	Statistic	Value	Units
2589M: Plastic Tray/ Pot/ Tub/ Cup, C: S	Per unit body weight	Total Population	All	All Foods	Mean	0.000143214	mg/kg bw
2673M: Glass Bottle, C: Crown Closure	Per unit body weight	Total Population	All	All Foods	Mean	5.26636e-005	mg/kg bw
3509M: Brick shaped beverage carton, C:	Per unit body weight	Total Population	All	All Foods	Mean	0.00118665	mg/kg bw
3676M: Flexible Wrapper/ Bag/ Pouch	Per unit body weight	Total Population	All	All Foods	Mean	0.00741322	mg/kg bw
4596M: Flexible Wrapper/ Bag/ Pouch, C:	Per unit body weight	Total Population	All	All Foods	Mean	6.95481e-005	mg/kg bw
6184M: Other beverage carton	Per unit body weight	Total Population	All	All Foods	Mean	0.000153063	mg/kg bw

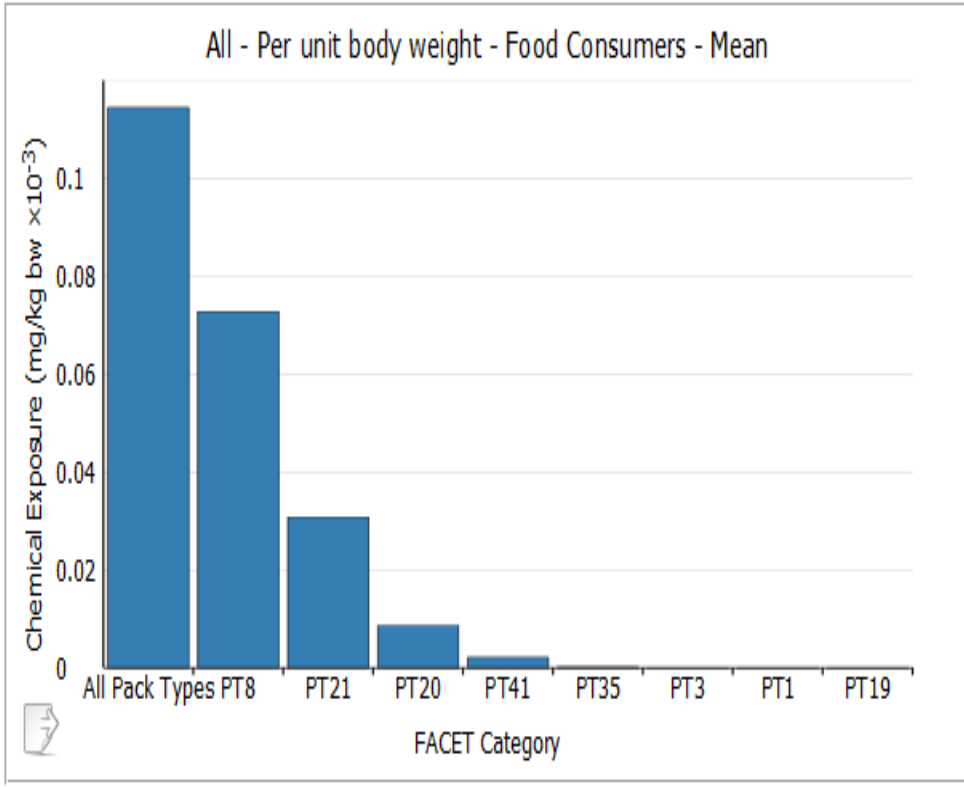
FACET

ile Changes New Help

By Food Category | By Pack Type

Home | Assessments | FACET Data | My Data | Results - Substa...





	Survey	Pack Type / Food	Pack Type Description	Intake Type	Consumer T...	FACET Category Co...	FACET Category Na...	Statistic	Value	Units
2489	UK NDNS 2000	PT41	M: Glass Jar, C: Metal Twist/ Lev	Per unit body weigh	Total Population	All	All Foods	Mean	2.0818e-(	mg/kg b
2500	UK NDNS 2000	PT41	M: Glass Jar, C: Metal Twist/ Lev	Per unit body weigh	Food Consumers	All	All Foods	Mean	2.0818e-(	mg/kg b
27569	UK NDNS 2000	PT35	M: Glass Bottle, C: Metal Twist/	Per unit body weigh	Total Population	All	All Foods	Mean	1.35131e-	mg/kg b
27580	UK NDNS 2000	PT35	M: Glass Bottle, C: Metal Twist/	Per unit body weigh	Food Consumers	All	All Foods	Mean	1.35131e-	mg/kg b
29241	UK NDNS 2000	PT3	M: Aerosol can, C: Plastic Other	Per unit body weigh	Total Population	All	All Foods	Mean	2.3641e-(	mg/kg b

Predictive Uses

Product Development

- Bringing new substances to market
- New packaging types/structures

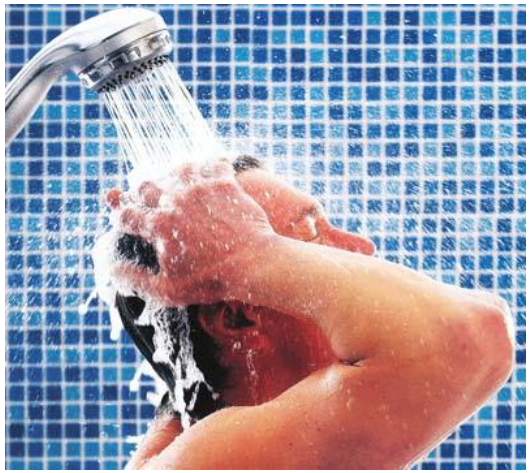
Risk Assessment

- NIAS
- Scenario analysis

How much fragrance gets on our skin and into our bodies?

FRAGRANCES

Daily Aggregate Exposure





Aggregate Exposure Modelling

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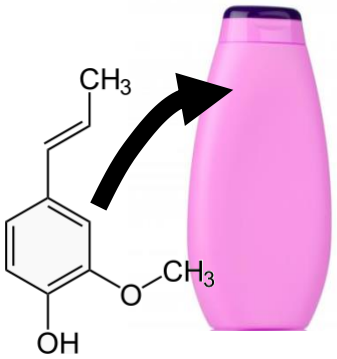
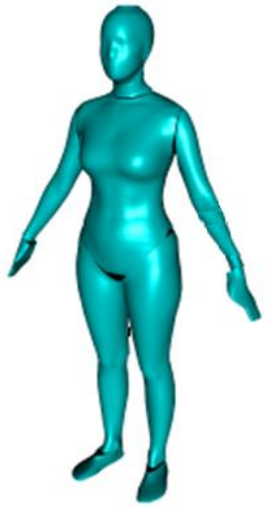
$$Agg\ Exp = \frac{Frequency \times Amount \times Retention \times Concentration}{Surface\ Area}$$

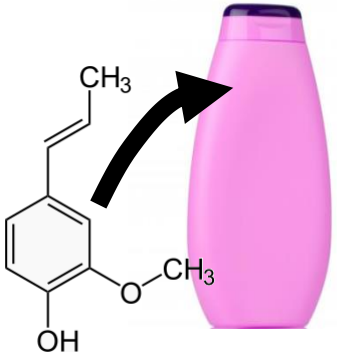
Aggregate Exposure Modelling

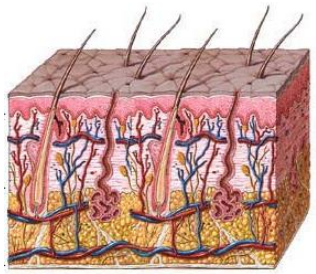


$$Agg\ Exp = \frac{Frequency \times Amount \times Retention \times Concentration}{Surface\ Area}$$



Aggregate Exposure Modelling

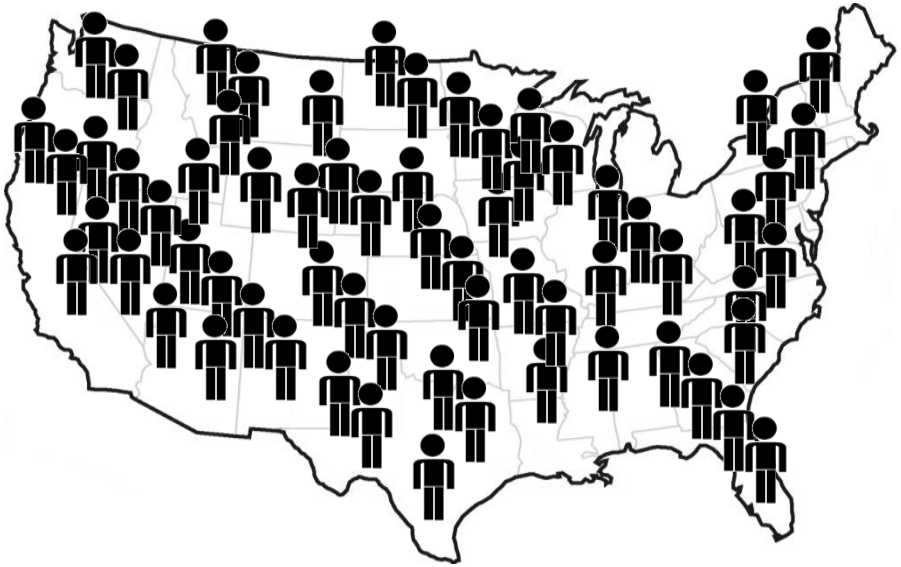




$$Agg\ Exp = \frac{Frequency \times Amount \times Retention \times Concentration \times Penetration}{Bodyweight}$$

Population Exposure Modelling

Creme GLOBAL



Frequency of Use

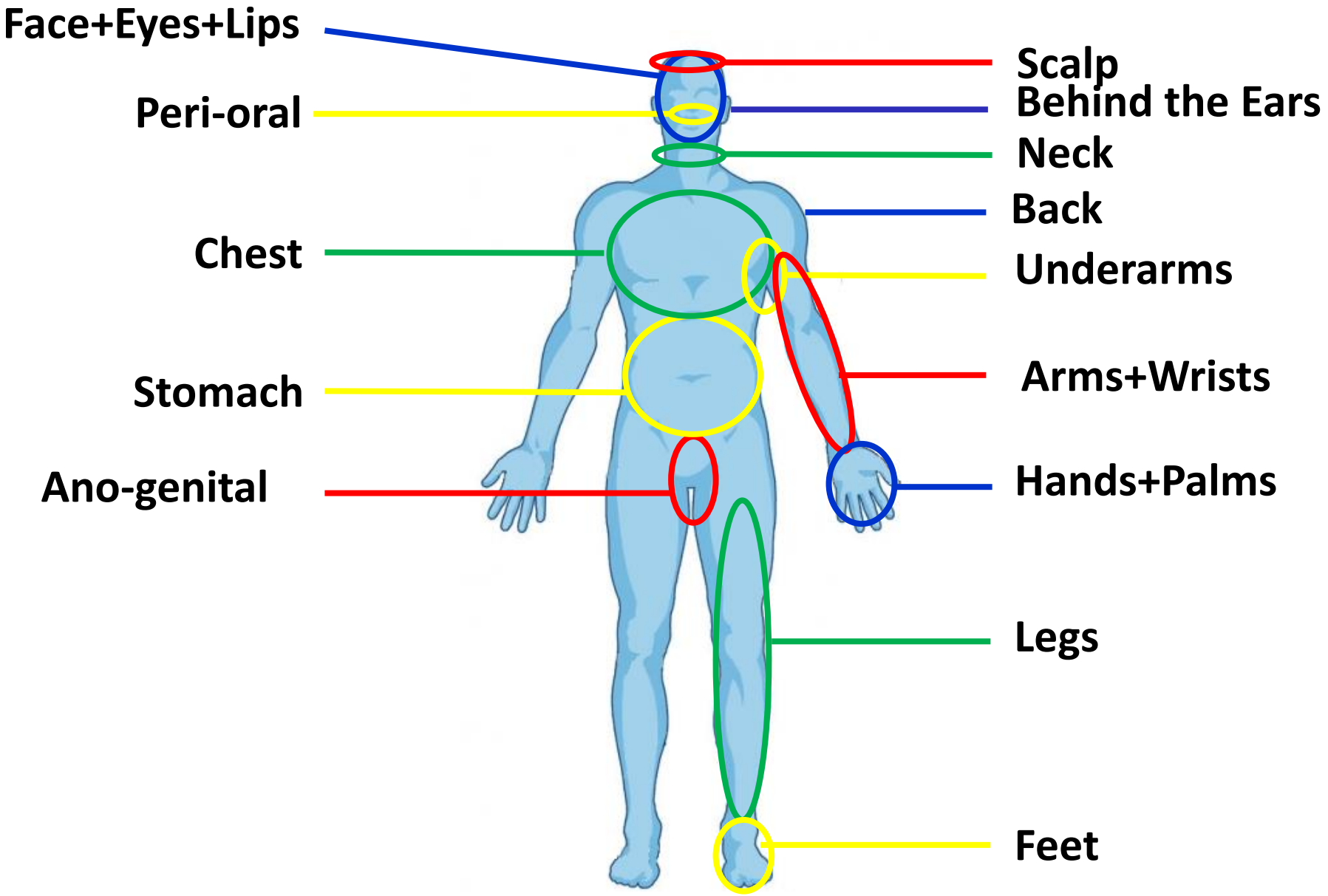
KANTAR WORLDPANEL

Online Consumption Diaries

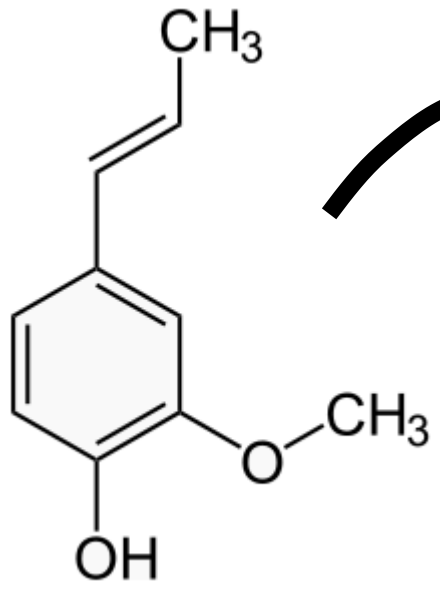




Application Sites



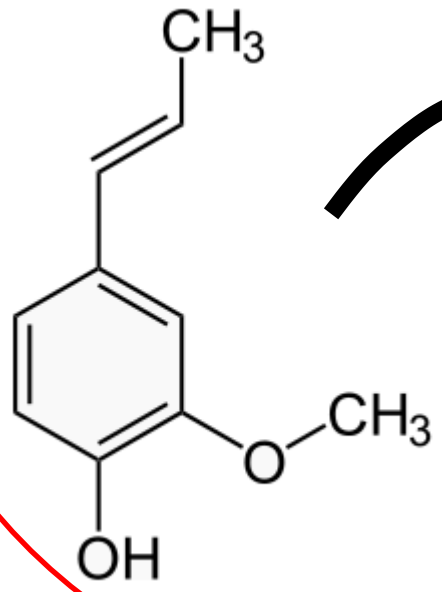
Fragrance Concentrations



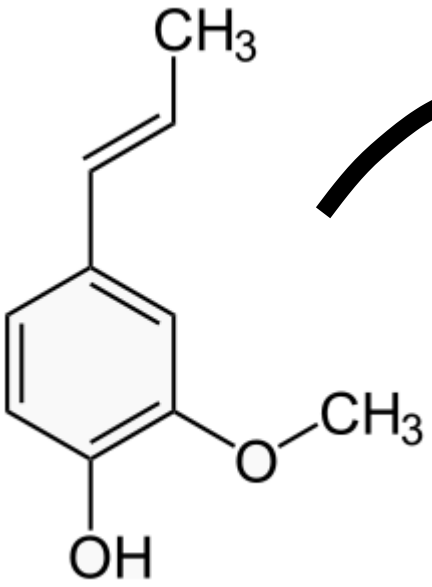
Fragrance Concentration

Creme GLOBAL

Fragrance Manufacturers



Fragrance Concentration



Consumer Product Companies

Survey 007

New File

Closing Date: June 10th, 2015

Please create a file for every fragrance that you wish to enter data for.

#	Fragrance	Created at	Updated at	Status		
1	799259-56-6 (RIFM ID: 7092-A2.12) *Cyperus articulatus oil (Essential oil by steam distill…*	15 May, 2015, 2:31 pm		Active	Edit	Delete
2	7775-00-0 *3-(p-Isopropylphenyl)propionaldehyde*	15 May, 2015, 2:31 pm		Active	Edit	Delete
3	7549-37-3 *Citral dimethyl acetal*	15 May, 2015, 2:31 pm		Active	Edit	Delete
4	7493-57-4 *Propyl phenethyl acetal*	15 May, 2015, 10:36 am		Active	Edit	Delete
5	72869-82-0 (RIFM ID: 1285-E2.30) *Lemongrass oil terpenes (Terpenes)*	15 May, 2015, 10:36 am		Active	Edit	Delete

100-51-6 Active

BenzylAlcohol

Save | Save and Exit | Save and Submit

Comments:

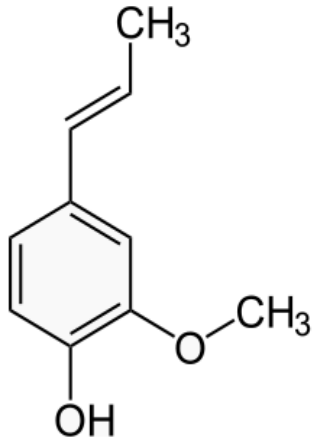
Click here to enter your comments.

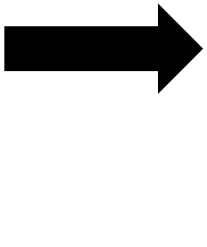
Errors:

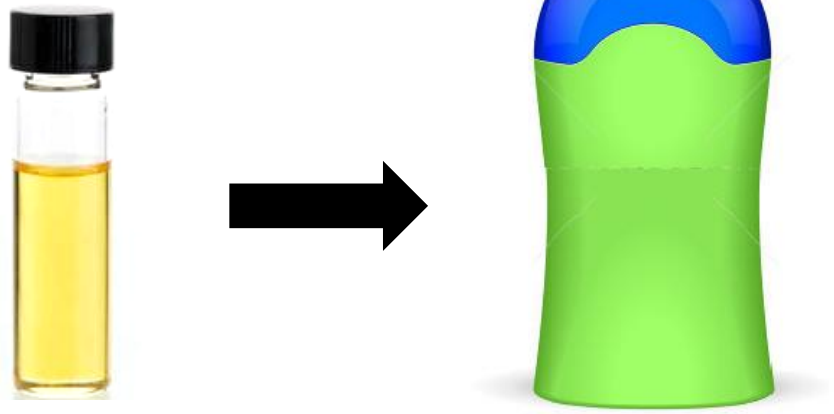
Your data contains 0 errors.

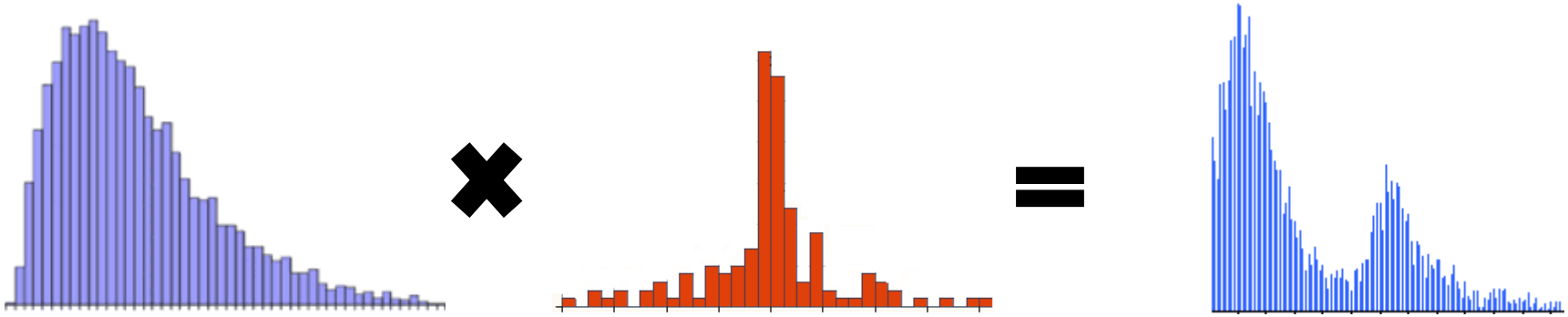
	BodyLotionMass	BodyLotionPrestige	DeoSpray	DeoRollOn	BodySpray	Toothpaste	Mouthwash
1	0.0100000	0.2000000	0.6640000	0.3320000	0.0100000	14	0.3330000
2	0.0010000		0.6900000	0.0100000	0.0011100		0.1110000
3	0.3000000		0.0100000	0.0010000			0.6611000
4	2		0.0010000	0.3000000			0.0880000
5	0.1110000		0.3000000				0.0666000
6	0.6611000		1.1000000				0.2220000
7			0.1110000				
8			0.6611000				
9			0.0880000				
10			0.0666000				
11			0.2220000				
12			0.0006644				
13			0.3300000				
14			0.0555000				
15			0.0010000				
16			0.0880000				
17			0.0666000				
18			0.2220000				
19			0.0215880				
20			0.3611000				
21			0.1440000				

Fragrance Concentration

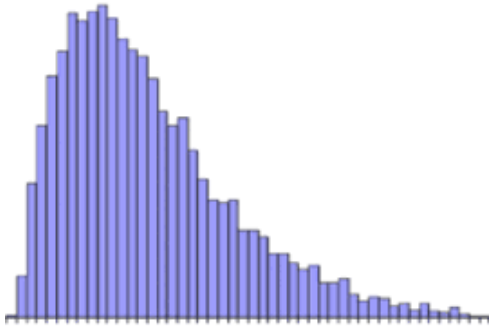


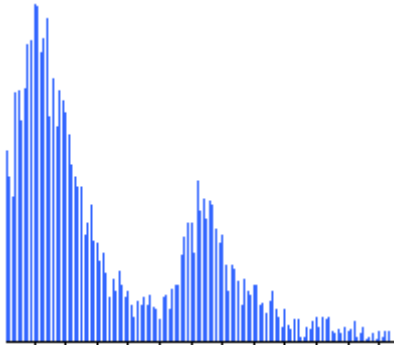




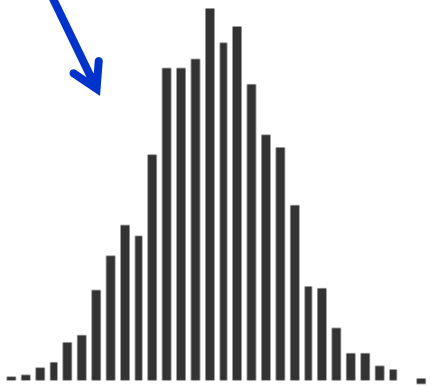


Aggregate Exposure Modelling





$$\text{Exposure} = \frac{Amount \times Retention \times Concentration \times Penetration}{Body\ Weight}$$



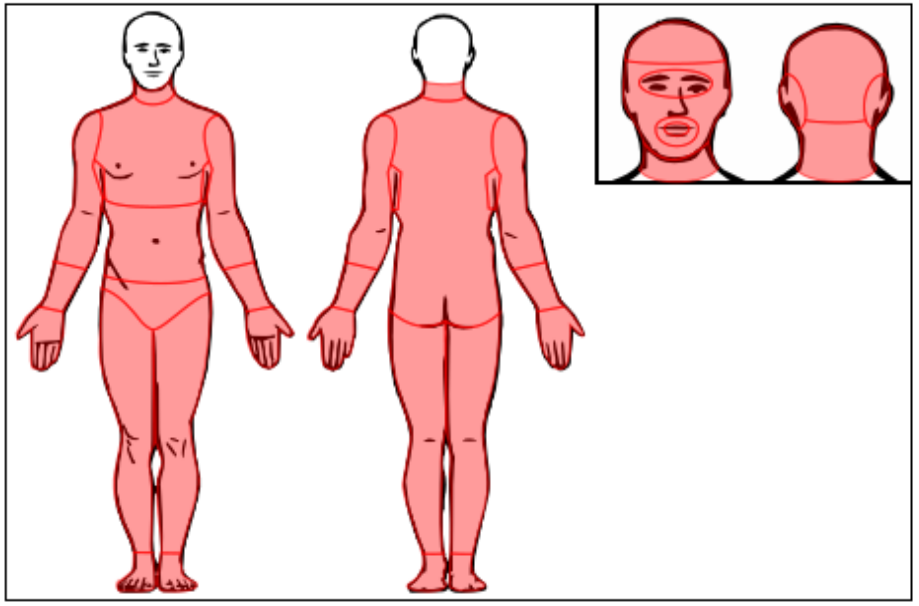
New Assessment Wizard

Select Body Parts

- Select Demographic
- Select Products
- Select Fragrances
- Select Body Parts
- Assessment Options
- Assessment Summary

Select All

- Scalp
- Face
- Eyes
- Lips
- Mouth
- Neck
- Behind Ears
- Chest
- Stomach
- Back
- Underarms
- Arms
- Wrists
- Hands
- Palms
- Intimate Parts
- Legs
- Feet



Number of Body Parts Selected: 18

Cancel <Previous Next>

Creme RIFM Fragrance Exposure Analysis

File Go Actions View Help

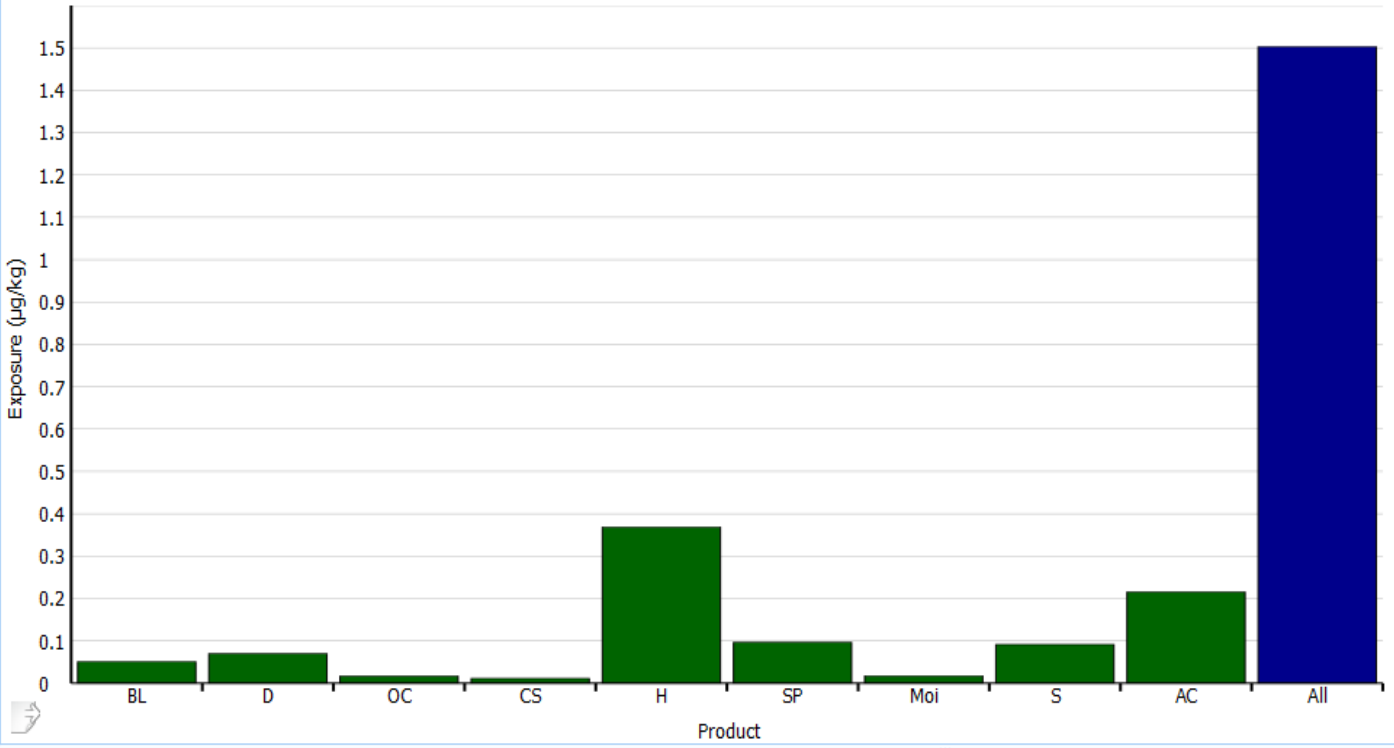
Account Settings (user3)

New Assessment New Optimisation Assessment By Product By Body Part

My Assessments New Assessment

Benzaldehyde

100-52-7 [100-52-7] - All Population - P95
Total Body (Systemic, Per Unit Bodyweight)



BL: BodyLotion
D: Deodorant
OC: OralCare
CS: CosmeticStyling
H: Hydroalcoholics
SP: ShowerProducts
Moi: Moisturizers
S: Soaps
AC: AirCare
All: All Assessed Products

Body Part: Total Body **Fragrance / Product:** 100-52-7 [100-52-7] **Calculation Type:** Acute (Max Day) **Exposure Type:** Total Body (Systemic, Per Unit Bodyweight)

	Product	Consumer Type	Statistic	Value	Units	Standard Error
4539	BodyLotion	All Population	P95	0.0508	µg/kg	0.0060
2475	Deodorant	All Population	P95	0.0697	µg/kg	0.0055
2460	OralCare	All Population	P95	0.0167	µg/kg	0.0009
5664	CosmeticStyling	All Population	P95	0.0111	µg/kg	0.0013
1977	Hydroalcoholics	All Population	P95	0.3685	µg/kg	0.0179

Creme RIFM Fragrance Exposure Analysis

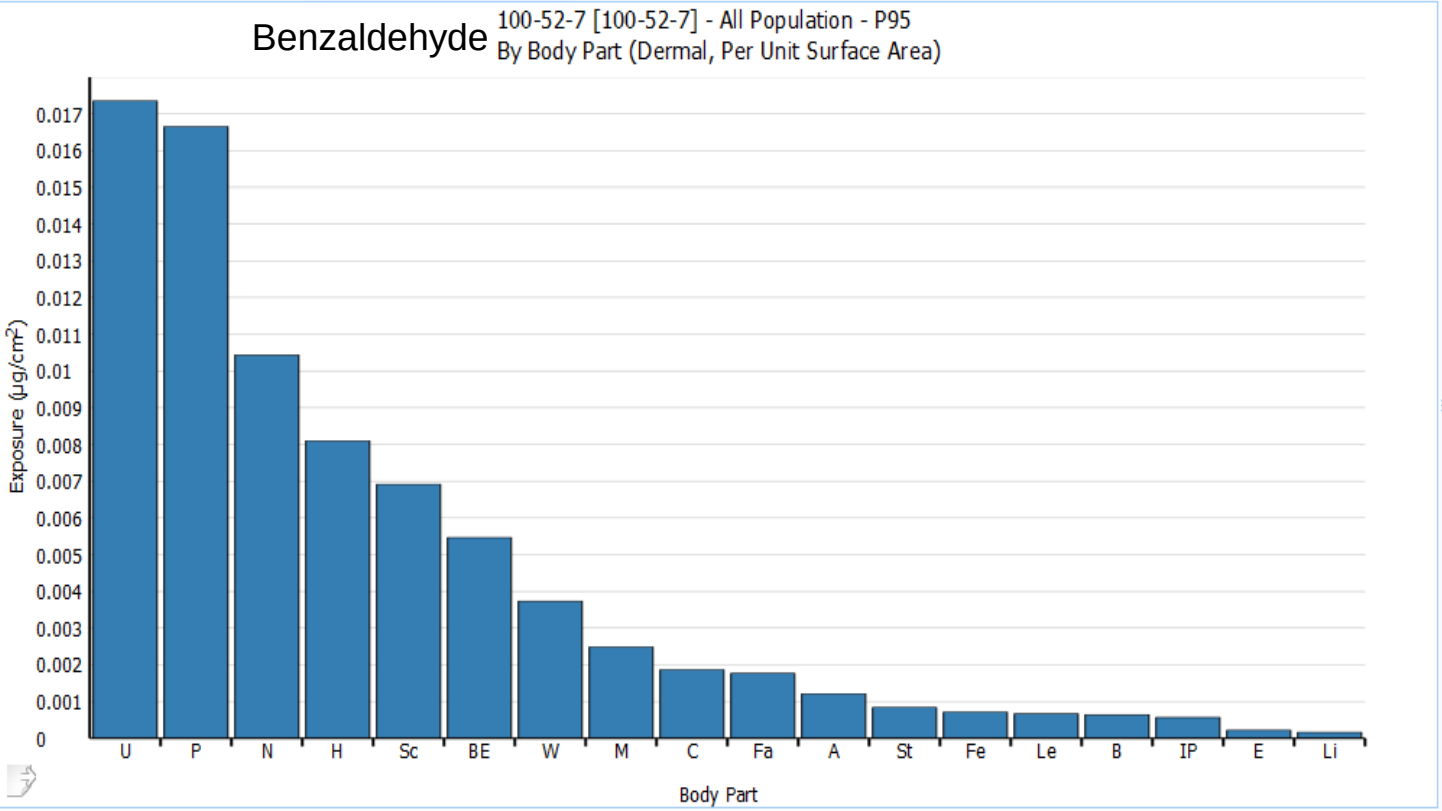
File Go Actions View Help

Account Settings (user3)

New Assessment New Optimisation Assessment

By Product By Body Part

My Assessments New Assessment



Sc: Scalp
Fa: Face
E: Eyes
Li: Lips
M: Mouth
N: Neck
BE: BehindEars
C: Chest
St: Stomach
B: Back
U: Underarms
A: Arms
W: Wrists
H: Hands
P: Palms
IP: IntimateParts
Le: Legs
Fe: Feet

Product: All Assessed Products **Fragrance / Product:** 100-52-7 [100-52-7] **Calculation Type:** Acute (Max Day) **Exposure Type:** By Body Part (Dermal, Per Unit Surface Area)

	Body Part	Consumer Type	Statistic	Value 1	Units	Standard Error
2847	Underarms	All Population	P95	0.0173	µg/cm²	0.0014
5325	Palms	All Population	P95	0.0167	µg/cm²	0.0006
2343	Neck	All Population	P95	0.0104	µg/cm²	0.0004
5094	Hands	All Population	P95	0.0081	µg/cm²	0.0005
6702	Scalp	All Population	P95	0.0069	µg/cm²	0.0002
1524	BehindEars	All Population	P95	0.0055	µg/cm²	0.0005

Predictive Intake Modelling

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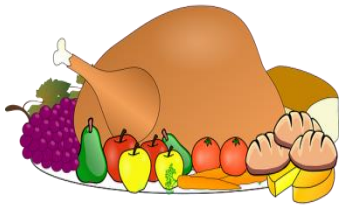

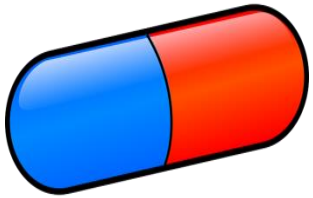

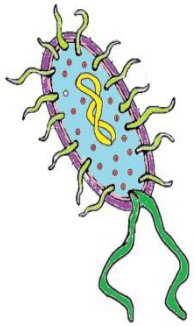

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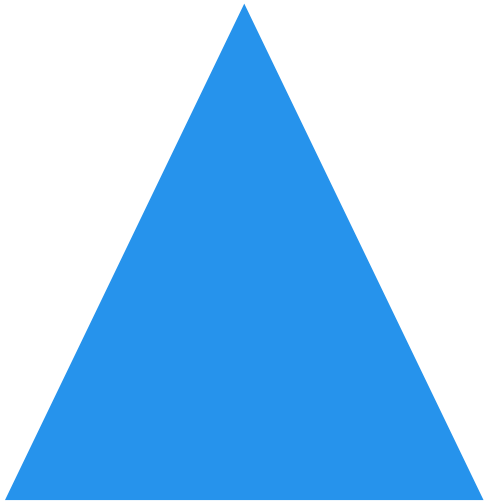
Data

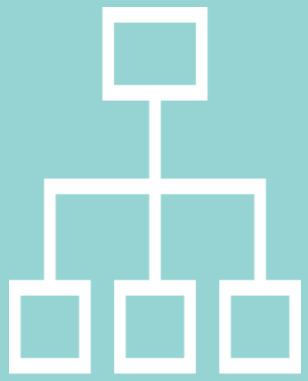


Data Science

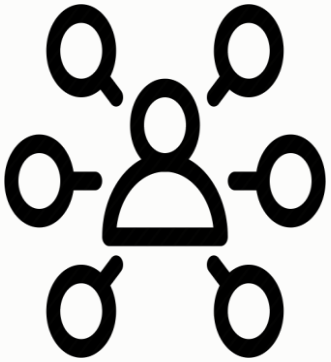
Decision Makers

Challenges

No Data, No Product



Workflow Broken



Expert Team Needed

No Communication,
No Acceptance

Deep Knowledge Needed

Ad Hoc Development Process

Solution

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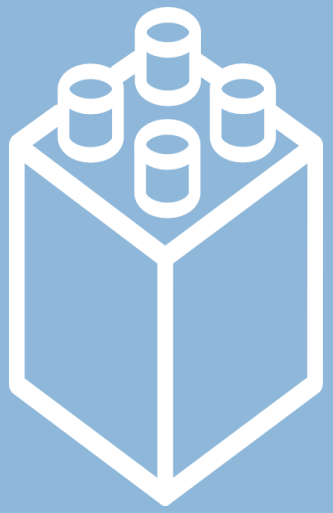
Data

Data Science

Decision Makers

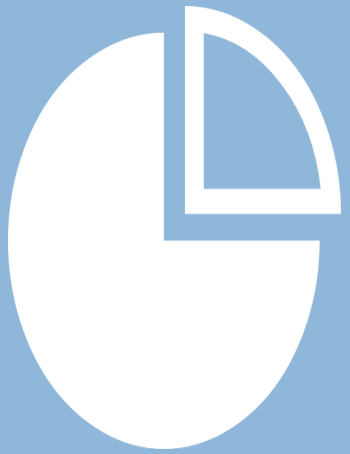
Connect

Deploy



Build

Collaborate



Analyse

Collaborate

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Ecosystem / Community

Collaboration Groups

Find Partners

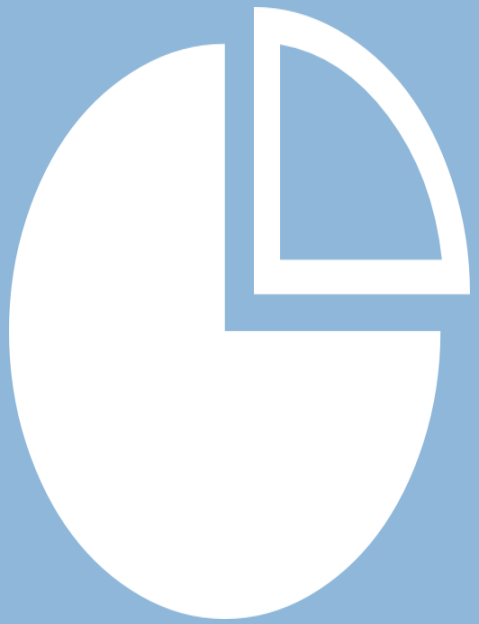
Find Customers

Buy / Sell Models

Buy / Sell Data Sets

Request Expertise

Analyse



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Curated Libraries

Custom Libraries

Statistical Toolkits

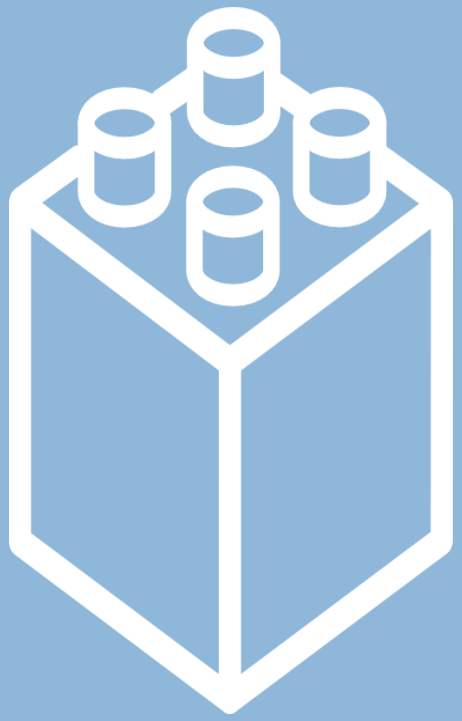
Finance Toolkits

Monte Carlo

Risk Analysis

Graphing / Visualisation

Build



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Quicker, Better, Easier

Curated Libraries

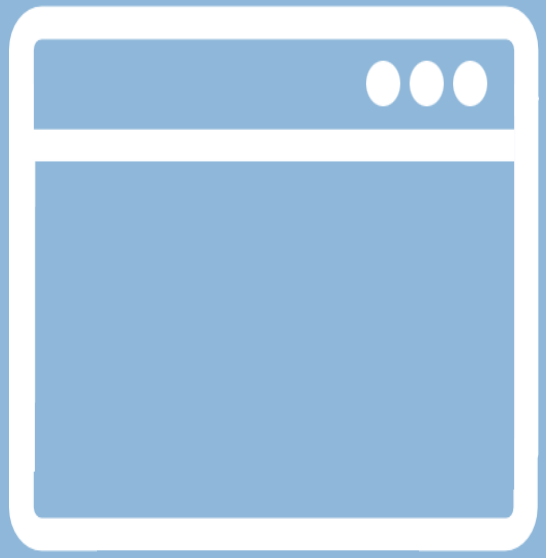
Custom Libraries

Quality Built In

Optimised

Documented

Deploy



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Deploy Quickly & Easily

Beautiful Interfaces

Share Models

Share Results

Collaborate

Connect

=

Datasets

Databases

Data APIs

Open Data

Third Party Data

API Services

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EXPERT MODELS

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EXPERT MODELS

Data Analytics Set Free

Expert Models for Decision Makers ™

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