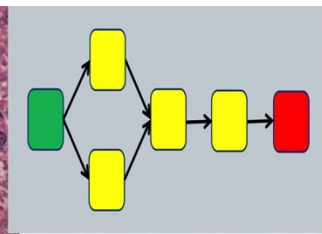
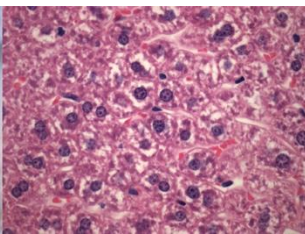
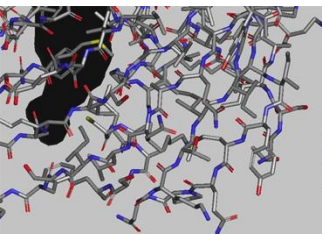




*Aggregate exposure to bisphenol A from food and
personal care products:
A hands-on training in PACEM Shiny and MCRA*

Cecile Karrer, Christiaan Delmaar, Bas Bokkers,
Konrad Hungerbühler, Natalie von Goetz

Eurotox 2018 – Continuing Education Course, Brussels, 2 September 2018



- Introduction of the PACEM model and its Shiny application
- Introduction of hands-on training with bisphenol A (BPA) case study



In PACEM Shiny: Modeling of BPA exposure from personal care products (PCPs)



Export of results for use in MCRA



In MCRA: Modeling of aggregate exposure to BPA from PCPs and food

Aggregate exposure assessment:

Considering exposure to one chemical via multiple exposure routes (here: oral dietary, oral PCPs, and dermal PCPs)



Probabilistic Aggregate Consumer Exposure Model

- Person-oriented model for calculating exposure to PCPs
- Developed by RIVM and ETH Zurich to simplify realistic exposure assessments
- Essential are product use data obtained from population surveys
- PACEM has been described and tested in different publications (2014,2015)

The probabilistic aggregate consumer exposure model (PACEM):
Validation and comparison to a lower-tier assessment for the cyclic siloxane D5



Tatsiana Dudzina ^a, Christiaan J.E. Delmaar ^b, Jacqueline W.H. Biesterbos ^c, Martine I. Bakker ^b, Bas G.H. Bokkers ^b, Paul T.J. Scheepers ^c, Jacqueline G.M. van Engelen ^b, Konrad Hungerbuehler ^a, Natalie von Goetz ^{a,*}

Validation of an aggregate exposure model for substances in consumer products: a case study of diethyl phthalate in personal care products

Christiaan Delmaar¹, Bas Bokkers¹, Wouter ter Burg¹ and Gerlienke Schuur¹

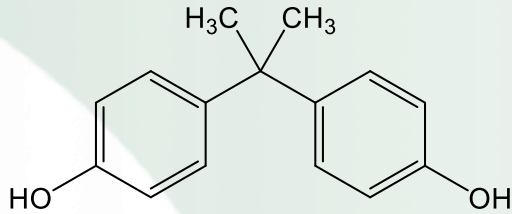
Aggregate exposure approaches for parabens in personal care products: a case assessment for children between 0 and 3 years old

Ilse Gosens¹, Christiaan J.E. Delmaar¹, Wouter ter Burg¹, Cees de Heer¹ and A. Gerlienke Schuur¹

- PACEM has always been available in the programming language R
 - Not very user friendly, only used by small number of people
- With the Shiny package, interactive applications can be built from R code
 - PACEM Shiny application has PACEM functionality in a user interface that is easier to use
- PACEM Shiny is a **beta** version
 - It is still under development and not working perfectly yet
 - Please let us know if you find bugs or have suggestions for improvement



BPA case study for hands-on training



Occurrence

Plasticizer for production of polycarbonate plastics (PC) and epoxy resins
→ Migration, diffusion: dietary products, cosmetics, dust, and air

Color developer in thermal paper
→ Receipts



Health effects

Endocrine disrupting substance

- Estrogenic activity
- Anti-androgenic activity
- Effects on steroid hormone synthesis

TDI 4 µg/kg bw/day

Regulation in EU

2011: EU-wide ban of PC babybottles and set migration limit from plastics

2015: Ban from food contact materials in France

let's get started



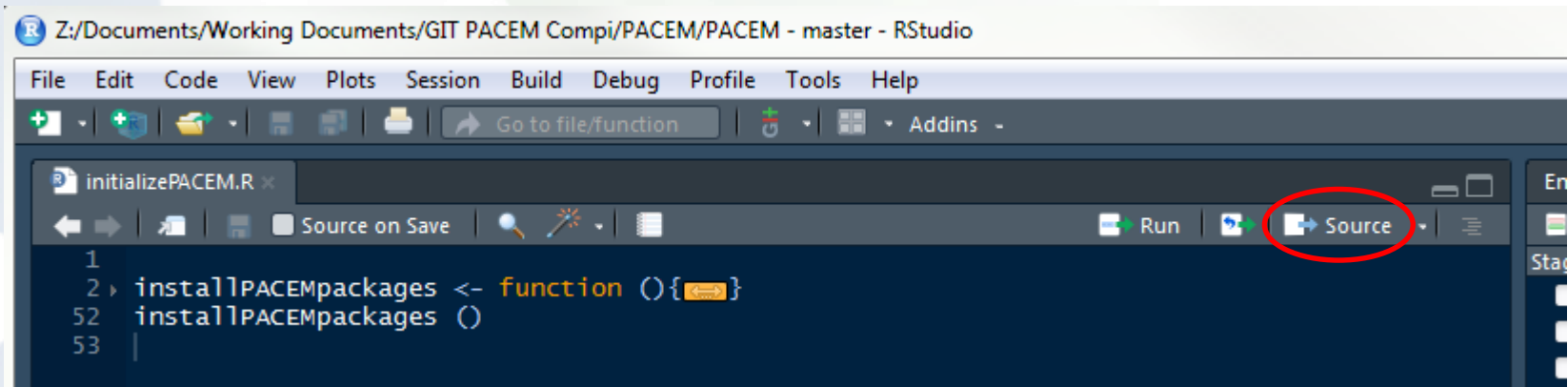
Please note:
All results shown are for illustration purposes
No risk assessment



Installation of R packages needed

Did everyone get the files from the USB stick?

1. Start R Studio
2. In R Studio, open the file 'initializePACEM.r' (folder PACEM)
3. Press the 'source' button

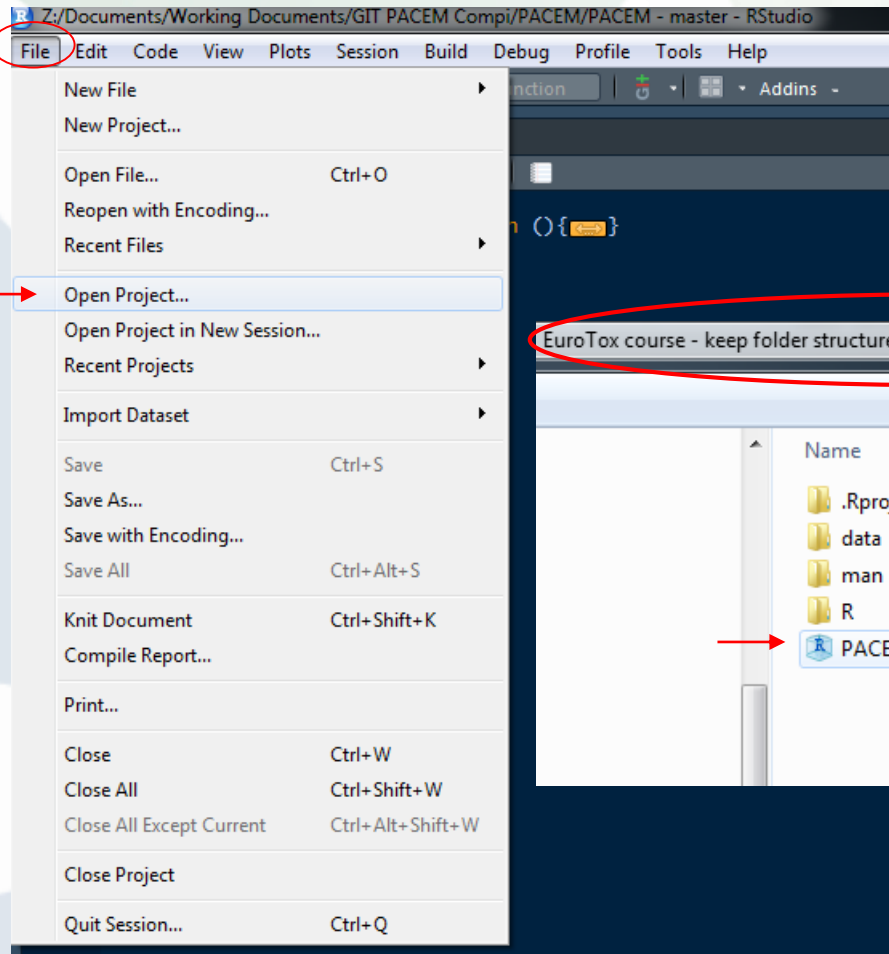


The screenshot shows the R Studio interface. The title bar reads 'Z:/Documents/Working Documents/GIT PACEM Compi/PACEM/PACEM - master - RStudio'. The menu bar includes File, Edit, Code, View, Plots, Session, Build, Debug, Profile, Tools, and Help. The toolbar contains various icons, including a 'Source' button which is circled in red. The editor window shows the following R code:

```
1  
2 > installPACEMpackages <- function () {  
52 installPACEMpackages ()  
53 |
```

Please note: the installation of packages in R only needs to be done once (per R version)

Installation of PACEM package (I)



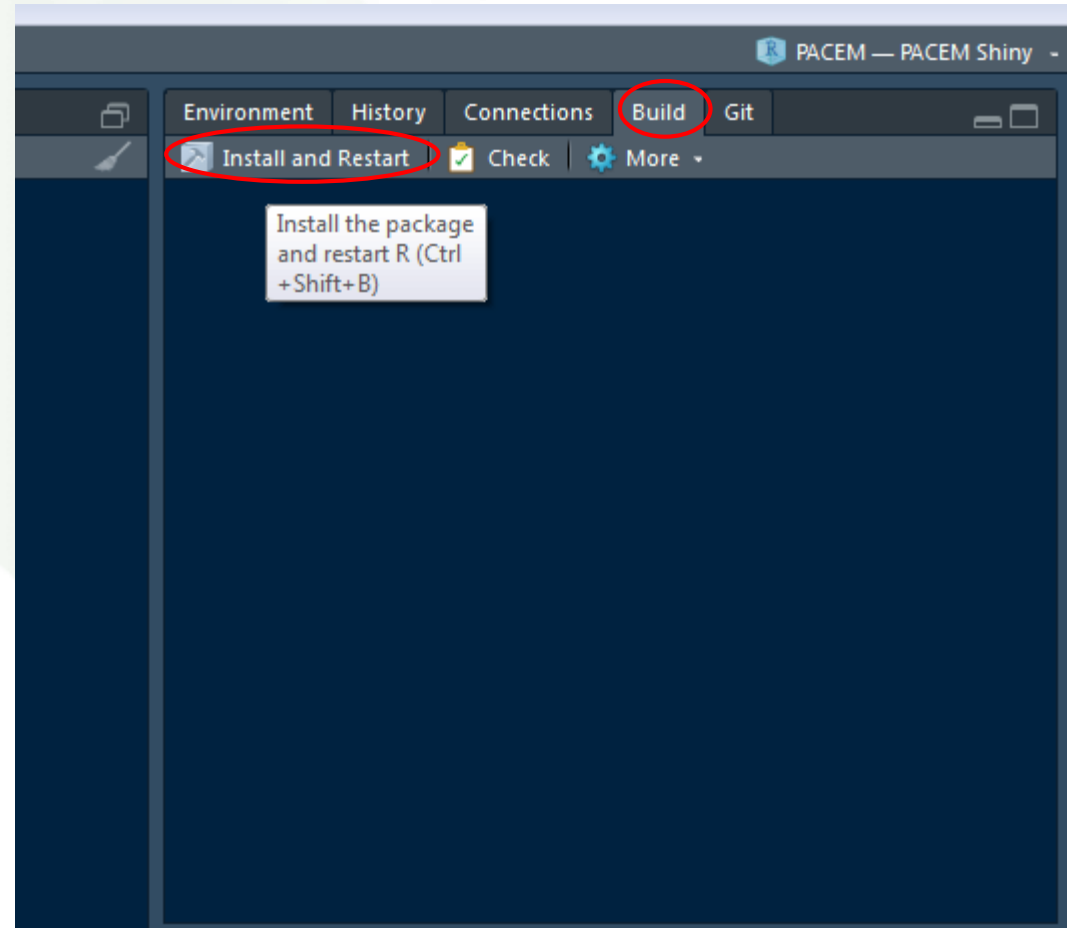
Still in R Studio, open the project 'PACEM' from the path indicated below

Please note: the installation of packages in R only needs to be done once (per R version)



Installation of PACEM package (II)

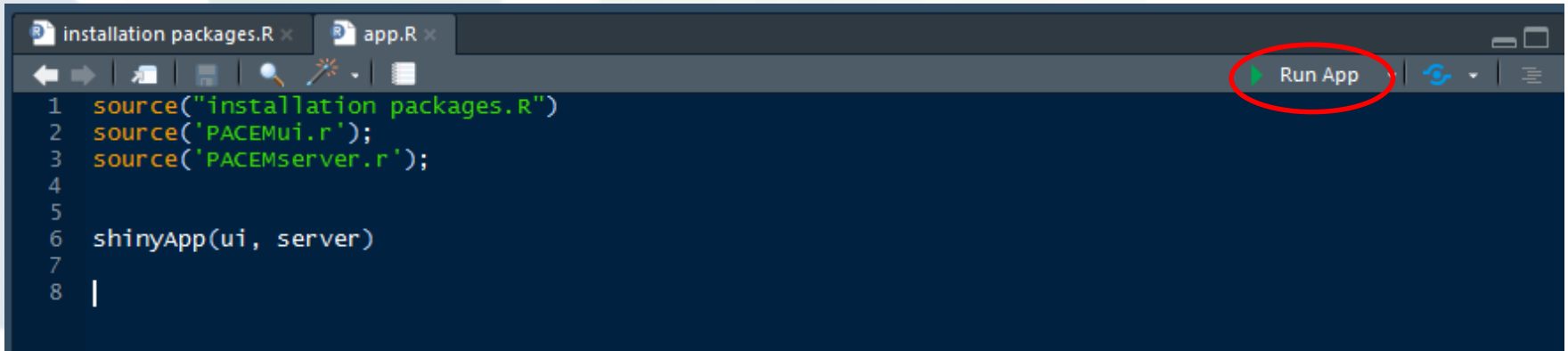
- click 'Install and Restart' in the 'Build' panel
- Wait until installation and restart is finished



Please note: the installation of packages in R only needs to be done once (per R version)

Run PACEM Shiny application

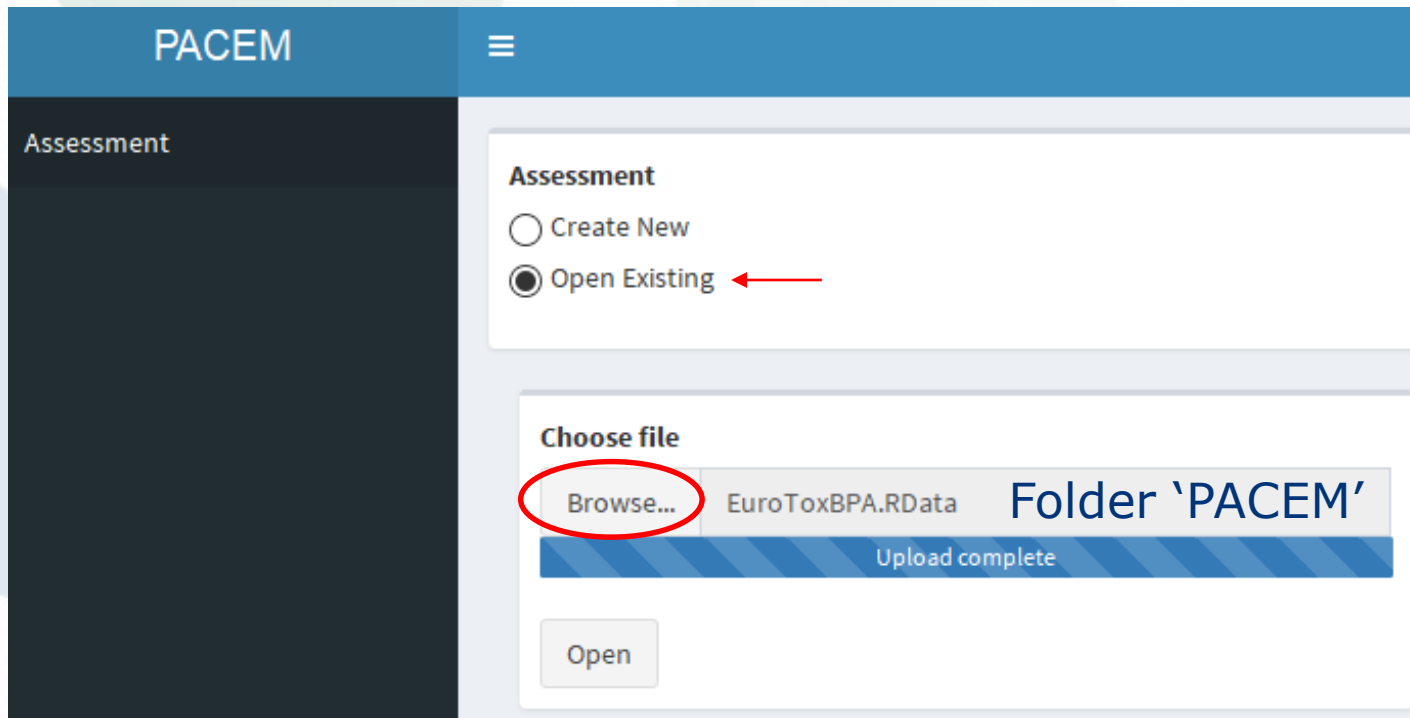
1. Still in R Studio, open the file 'app.R' (in PACEM Shiny\PACEM\shiny)
2. Press the 'run app' button



```
installation packages.R × app.R ×
← → ↻ 🔍 📄
1 source("installation packages.R")
2 source('PACEMui.r');
3 source('PACEMserver.r');
4
5
6 shinyApp(ui, server)
7
8 |
```



Open existing assessment «EuroToxBPA»



The screenshot shows the PACEM web interface. On the left is a dark sidebar with the word 'Assessment' at the top. The main content area has a blue header with 'PACEM' and a menu icon. Below the header, there are two sections. The first section, titled 'Assessment', contains two radio button options: 'Create New' and 'Open Existing'. A red arrow points to the 'Open Existing' option. The second section, titled 'Choose file', shows a file upload progress bar. The progress bar is partially filled with blue and contains the text 'EuroToxBPA.RData' and 'Folder 'PACEM''. A blue bar at the bottom of the progress bar says 'Upload complete'. Below the progress bar is a button labeled 'Open'. The 'Browse...' button in the file selection area is circled in red.



PACEM



✓ Assessment

Survey and Endpoint

Personal Care Products (PCPs) Survey

Dutch survey (Biesterbos 2013) ▼

Include household cleaning products

← Do not tick this

Please note: The Swiss survey includes information on both PCPs and HPs. For the Dutch and the mixed European surveys, another survey called EPHECT will be included to model exposure from HPs.

Exposure Metric

systemic exposure ▼

Save as

Save & continue



Estimation of intake and uptake of bisphenols and triclosan from personal care products by dermal contact☆

Shaoyou Lu ^{a,b}, Yuling Yu ^c, Lu Ren ^a, Xiaolan Zhang ^c, Guihua Liu ^a, Yingxin Yu ^{c,*}

^a Shenzhen Center for Disease Control and Prevention, Shenzhen 518055, China

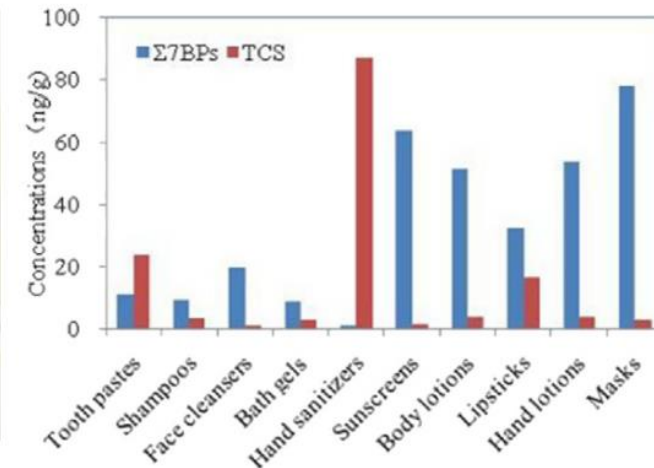
^b State Key Laboratory of Organic Geochemistry, Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, Guangzhou 510640, China

^c Institute of Environmental Pollution and Health, School of Environmental and Chemical Engineering, Shanghai University, Shanghai 200444, China

HIGHLIGHTS

- Occurrence and distribution of BPs and TCS in personal care products were studied.
- High levels of BPF indicated the widely use of BPF as a substitute for BPA.
- The EDU of targets factored dermal absorption rates were markedly lower than the EDI.
- The human exposure to BPA from PCPs via dermal contact cannot be neglected.

GRAPHICAL ABSTRACT



- ✓ Assessment
 - ✓ Survey and Endpoint
 - ✓ Concentration Data
 - ✓ Exposure Fractions
 - ✓ Simulation
- Analysis

Concentration data

Please enter product concentrations in ng/g

	Product name	Sample size	Distribution	Fraction without substance	Parameter 1	Parameter 2	Parameter 3	Parameter 4
1	Aftershave balsam	1000	trunc lognorm	0.2730	4.67	3.85	18.10	200.37
2	Aftershave spray		NA					
3	Aftersun cream	1000	trunc lognorm	0.5830	4.56	4.02	18.10	206.84
4	Bathingfoam	1000	uniform	0.9520	18.10	60.40		
5	Bathingoil	1000	uniform	0.9520	18.10	60.40		
6	Bodylotion milk	1000	uniform	0.7500	18.10	60.40		
7	Bronzing cream	1000	trunc lognorm	0.5830	4.56	4.02	18.10	206.84
8	Cleansing lotion	1000	trunc lognorm	0.8890	4.10	3.41	18.10	121.09
9	Conditioner	1000	uniform	0.8000	18.10	60.40		
10	Deo cream		NA					
11	Deo roller stick		NA					
12	Deo spray		NA					
13	Deo tissue		NA					
14	Shower gel	1000	uniform	0.9520	18.10	60.40		
15	Eyebrow pencil		NA					
16	Eyeliner pencil		NA					
17	Eye shadow		NA					
18	Face day cream	1000	trunc lognorm	0.2730	4.67	3.85	18.10	200.37
19	Face night cream	1000	trunc lognorm	0.2730	4.67	3.85	18.10	200.37
20	Hair mousse		NA					
21	Hair gel		NA					
22	Hair lotion		NA					
23	Hairspray		NA					
24	Hair wax		NA					
25	Hand cream	1000	uniform	0.4710	18.10	60.40		
26	Lip balm	1000	uniform	0.0000	18.10	60.40		
27	Lip pencil		NA					
28	Lipstick	1000	uniform	0.0000	18.10	60.40		
29	Liquid foundation		NA					
30	Makeup remover		NA					
31	Mascara		NA					
32	Nail polish feet		NA					
33	Nail polish hands		NA					
34	Nail polish remover		NA					
35	Perfume spray		NA					
36	Rouge powder		NA					
37	Shampoo	1000	uniform	0.8000	18.10	60.40		
38	Shaving foam		NA					
39	Shaving gel		NA					
40	Shaving oil		NA					
41	Sun cream	1000	trunc lognorm	0.5830	4.56	4.02	18.10	206.84
42	Toothpaste		NA					

Parameter values depend on the distributions chosen

	Uniform	Trunc lognorm
Par 1	Minimum	Nat log (mean)
Par 2	Maximum	Nat log (std dev)
Par 3	-	Minimum
Par 4	-	Maximum

Concentration data

Please enter product concentrations in ng/g

	Product name	Sample size	Distribution	Fraction without substance	Parameter 1	Parameter 2	Parameter 3	Parameter 4
1	Aftershave balsam	1000	trunc lognorm ▾	0.2730	4.67	3.85	18.10	200.37
2	Aftershave spray		NA ▾					
3	Aftersun cream	1000	trunc lognorm ▾	0.5800	4.50	4.00	18.00	207.00
4	Bathingfoam	1000	uniform ▾	0.9500	18.00	60.00		
5	Bathingoil	1000	uniform ▾	0.9520	18.10	60.40		
6	Bodylotion milk	1000	uniform ▾	0.7500	18.10	60.40		
7	Bronzing cream	1000	trunc lognorm ▾	0.5830	4.56	4.02	18.10	206.84
8	Cleansing lotion	1000	trunc lognorm ▾	0.8890	4.10	3.41	18.10	121.09
9	Conditioner	1000	uniform ▾	0.8000	18.10	60.40		

Only these lines have not been filled yet

Fraction of BPA from a certain product, to which the individual is actually (here: externally) exposed to

Product measured	Product survey	EF dermal	EF oral	Reasoning
Sunscreen	Sunscreen, after-sun cream, bronzing cream	1	0	Reasonable worst-case stay-on skin scenario
Body lotion	Body lotion			
Hand lotion	Hand cream			
Face mask	Aftershave balsam, face cream day & night			
Face cleanser	Cleansing lotion	0.01	0	1 % of the product stays on skin after rinsing
Shampoo	Shampoo & conditioner			
Bath gel	Shower gel	0.005	0	Accounting for dilution and rinsing afterwards
	Bathing foam			
	Bathing oil			
Lipstick	Lipstick	0.1	0.9	Reasonable worst-case assumption
	Lipbalm			

- ✓ Assessment
- ✓ Survey and Endpoint
- ✓ Concentration Data
- ✓ Exposure Fractions
- ✓ Simulation

Analysis

Exposure fractions

	Product name	EF dermal	EF inhalation	EF oral
1	Aftershave balsam	1.0000		0.0000
2	Aftershave spray			
3	Aftersun cream	1.0000		0.0000
4	Bathingfoam	0.0050		0.0000
5	Bathingoil	0.0050		0.0000
6	Bodylotion milk	1.0000		0.0000
7	Bronzing cream	1.0000		0.0000
8	Cleansing lotion	0.0100		0.0000
9	Conditioner	0.0100		0.0000
10	Deo cream			
11	Deo roller stick			
12	Deo spray			
13	Deo tissue			
14	Shower gel	0.0100		0.0000
15	Eyebrow pencil			
16	Eyeliners pencil			
17	Eye shadow			
18	Face day cream	1.0000		0.0000
19	Face night cream	1.0000		0.0000
20	Hair mousse			
21	Hair gel			
22	Hair lotion			
23	Hairspray			
24	Hair wax			
25	Hand cream	1.0000		0.0000
26	Lip balm	0.1000		0.9000
27	Lip pencil			
28	Lipstick	0.1000		0.9000
29	Liquid foundation			
30	Makeup remover			
31	Mascara			
32	Nail polish feet			
33	Nail polish hands			
34	Nail polish remover			
35	Perfume spray			
36	Rouge powder			
37	Shampoo	0.0100		0.0000
38	Shaving foam			
39	Shaving gel			
40	Shaving oil			
41	Sun cream	1.0000		0.0000
42	Toothpaste			



Exposure fractions

	Product name	EF dermal	EF inhalation	EF oral
1	Aftershave balsam	1.0000		0.0000
2	Aftershave spray			
3	Aftersun cream	1.0000		0.0000
4	Bathingfoam	0.0050		0.0000
5	Bathingoil	0.0050		0.0000
6	Bodylotion milk	1.0000		0.0000
7	Bronzing cream	1.0000		0.0000
8	Cleansing lotion	0.0100		0.0000
9	Conditioner	0.0100		0.0000
10	Deo cream			
11	Deo roller stick			
12	Deo spray			
13	Deo tissue			
14	Shower gel	0.0100		0.0000
15	Eyebrow pencil			
16	Eveliner pencil			

Only these lines have not been filled yet



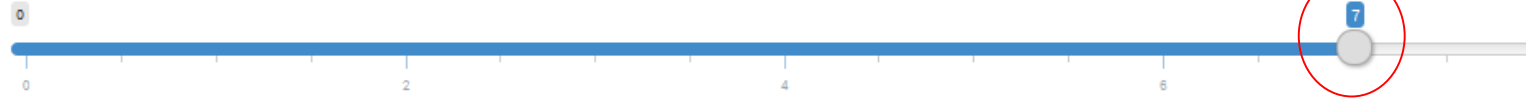
Simulation settings

PACEM



- ✓ Assessment
 - ✓ Survey and Endpoint
 - ✓ Concentration Data
 - ✓ Exposure Fractions
 - ✓ Simulation
- Analysis

Number of exposure days



Number of women

Number of men

Save as

Save & simulate

Save results to file? Please note: This could increase the file size significantly. ←





- ✓ Assessment
- ✓ Survey and Endpoint
- ✓ Concentration Data
- ✓ Exposure Fractions
- ✓ Simulation
- Analysis

Output analysis options

Your exposure simulation has finished.
Duration of model run: 1.54 min
for modeling exposure for 5000 women and 5000 men in 7 days.

Select exposure measure

acute

Select population

only exposed individuals

Select products

all products

Exposure routes

- dermal
 - oral
 - inhalation
 - total
-
- Create MCRA output

Percentiles to display in table

0.01

0.05

0.10

0.25

0.50

0.75

Add more fields

Display results



PACEM ☰

- ✓ Assessment
- ✓ Survey and Endpoint
- ✓ Concentration Data
- ✓ Exposure Fractions
- ✓ Simulation
- ✓ Analysis
- ✓ Results
- ✓ MCRA - settings

Summary Plots Simulated data

Assessment results

Results for the exposed individuals. 70.72 % of the total population is exposed.

Table of percentiles

systemic exposure in ng/kg

route	0.01	0.05	0.10	0.25	0.50	0.75	0.90	0.95	0.99
dermal	0.00026	0.0011	0.010	0.19	0.6826	2.3234	8.595	14.768	36.271
oral	0.00000	0.0000	0.000	0.00	0.0015	0.0078	0.018	0.026	0.062
total	0.00225	0.0066	0.015	0.19	0.6859	2.3311	8.607	14.813	36.277

Results are for illustration purposes - No risk assessment
EuroTox CEC – 2 Sept, 2018



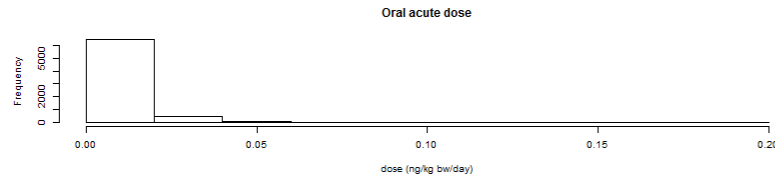
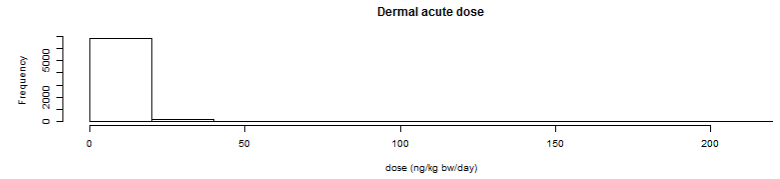
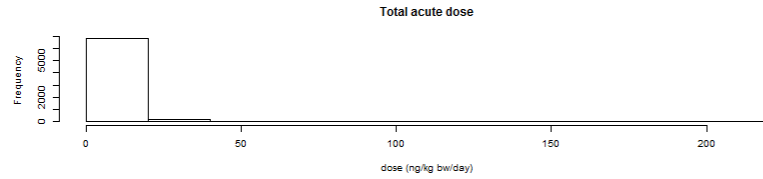
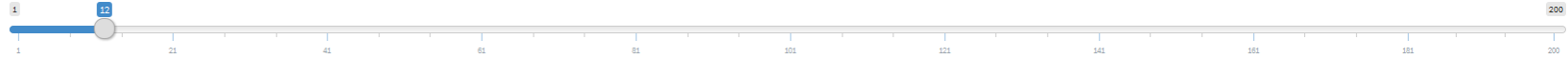
Result (II)

- ✓ Assessment
- ✓ Survey and Endpoint
- ✓ Concentration Data
- ✓ Exposure Fractions
- ✓ Simulation
- ✓ Analysis
- ✓ Results
- ✓ MCRA - settings

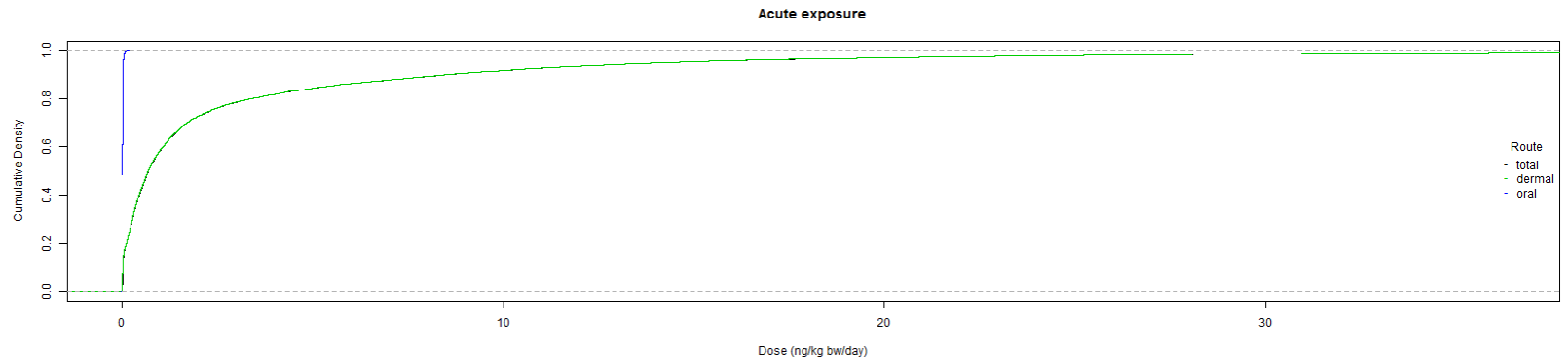
Summary Plots Simulated data

Histogram

Bins of histogram



Cumulative density function



Scale of x-axis

linear

Results are for illustration purposes - No risk assessment

EuroTox CEC - 2 Sept, 2018

This project is funded by the Horizon 2020 Framework Programme of the European Union



Results (III)

PACEM

- Assessment
- Survey and Endpoint
- Concentration Data
- Exposure Fractions
- Simulation
- Analysis
- Results
- MCRA - settings

Summary Plots Simulated data

Save simulation results please add '.csv' after the file name

Detailed simulation results

Show 10 entries Search:

product_name	person_id	survey_id	body_weight	gender	age	frequency	day	frequency_on_day	amount	fraction	dermal	oral	total
Aftershave_balsam	31200	96	85	male	35	0.263	12	1	2.050000	29.4	0.707000	0	0.707000
Aftershave_balsam	32700	197	98	male	49	0.253	7	1	0.000981	29.4	0.000294	0	0.000294
Aftershave_balsam	26800	73	85	male	57	1.000	7	1	0.600000	87.2	0.615000	0	0.615000
Aftershave_balsam	26800	73	85	male	57	1.000	9	1	0.713000	87.2	0.731000	0	0.731000
Aftershave_balsam	26800	73	85	male	57	1.000	1	1	0.894000	87.2	0.917000	0	0.917000
Aftershave_balsam	26800	73	85	male	57	1.000	10	1	0.534000	87.2	0.548000	0	0.548000
Aftershave_balsam	26800	73	85	male	57	1.000	12	1	1.320000	87.2	1.360000	0	1.360000
Aftershave_balsam	26800	73	85	male	57	1.000	8	1	1.240000	87.2	1.270000	0	1.270000
Aftershave_balsam	26800	73	85	male	57	1.000	6	1	0.944000	87.2	0.969000	0	0.969000
Aftershave_balsam	12500	234	79	male	51	1.000	10	1	1.280000	39.6	0.641000	0	0.641000

Showing 1 to 10 of 82,904 entries

Previous 1 2 3 4 5 ... 8291 Next

Results are for illustration purposes - No risk assessment
EuroTox CEC – 2 Sept, 2018



Export to MCRA (I)

PACEM ☰

- ✓ Assessment
- ✓ Survey and Endpoint
- ✓ Concentration Data
- ✓ Exposure Fractions
- ✓ Simulation
- ✓ Analysis
- ✓ Results
- ✓ MCRA - settings

Stratification and settings

Compound ID as specified in MCRA

Stratify by gender

yes no

Results are estimates for

internal exposure external exposure

Please specify non-dietary absorption factors

dermal

oral

inhalation

Create MCRA tables



PACEM



- ✓ Assessment
- ✓ Survey and Endpoint
- ✓ Concentration Data
- ✓ Exposure Fractions
- ✓ Simulation
- ✓ Analysis
- ✓ Results
- ✓ MCRA - settings
- ✓ MCRA- export

Overview

Table NonDietarySurveys

Table NonDietarySurveyProperties

Table NonDietaryExposures

Table NonDietaryAbsorptionFactors

To import non-dietary exposure estimates into MCRA, the following tables need to be provided.



Export to MCRA (III)

PACEM



- ✓ Assessment
- ✓ Survey and Endpoint
- ✓ Concentration Data
- ✓ Exposure Fractions
- ✓ Simulation
- ✓ Analysis
- ✓ Results
- ✓ MCRA - settings
- ✓ MCRA- export


Overview

Table NonDietarySurveys

Table NonDietarySurveyProperties

Table NonDietaryExposures

Table NonDietaryAbsorptionFactors

 Download please add '.csv' after the file name

idNonDietarySurvey	Description	NonDietaryIntakeUnit	PercentageZeros
1	PACEM output 2018-08-14	nanogram/day	0.00
2	PACEM output 2018-08-14	nanogram/day	0.00




Export to MCRA (IV)

PACEM

- Assessment
- Survey and Endpoint
- Concentration Data
- Exposure Fractions
- Simulation
- Analysis
- Results
- MCRA - settings
- MCRA- export

Overview Table NonDietarySurveys **Table NonDietarySurveyProperties** Table NonDietaryExposures Table NonDietaryAbsorptionFactors

 Download please add '.csv' after the file name

IndividualPropertyName	idNonDietarySurvey	IndividualPropertyTextValue	IndividualPropertyDoubleValueMin	IndividualPropertyDoubleValueMax
Gender	1	female	0.00	0.00
Gender	2	male	0.00	0.00



Export to MCRA (V)

PACEM

- Assessment
- Survey and Endpoint
- Concentration Data
- Exposure Fractions
- Simulation
- Analysis
- Results
- MCRA - settings
- MCRA - export

Overview | Table NonDietarySurveys | Table NonDietarySurveyProperties | Table NonDietaryExposures | Table NonDietaryAbsorptionFactors

Download Please add '.csv' after the file name

Show 10 entries

idIndividual	idNonDietarySurvey	idSubstance	Dermal	Oral	Inhalation
PACEM_1	2	RF-00000482-ORG	165.827903	0.0000000	0
PACEM_2	2	RF-00000482-ORG	21.202944	0.0000000	0
PACEM_3	2	RF-00000482-ORG	11.672759	0.0000000	0
PACEM_4	2	RF-00000482-ORG	187.253230	0.4585409	0
PACEM_5	2	RF-00000482-ORG	3.735879	0.0000000	0
PACEM_6	2	RF-00000482-ORG	88.193928	0.0000000	0
PACEM_7	2	RF-00000482-ORG	30.217088	0.0000000	0
PACEM_8	2	RF-00000482-ORG	37.044249	0.0000000	0
PACEM_9	2	RF-00000482-ORG	18.070476	0.0000000	0
PACEM_10	2	RF-00000482-ORG	5.118172	0.0000000	0

Showing 1 to 10 of 10,000 entries

Previous 1 2 3 4 5 ... 1000 Next

Results are for illustration purposes - No risk assessment

EuroTox CEC – 2 Sept, 2018



Export to MCRA (VI)

PACEM



- ✓ Assessment
- ✓ Survey and Endpoint
- ✓ Concentration Data
- ✓ Exposure Fractions
- ✓ Simulation
- ✓ Analysis
- ✓ Results
- ✓ MCRA - settings
- ✓ MCRA- export


Overview

Table NonDietarySurveys

Table NonDietarySurveyProperties

Table NonDietaryExposures

Table NonDietaryAbsorptionFactors

 Download

please add '.csv' after the file name

idNonDietarySurvey	idCompound	DermalAbsorptionFactor	OralAbsorptionFactor	InhalationAbsorptionFactor
1	RF-00000482-ORG	0.20	1	1
2	RF-00000482-ORG	0.20	1	1



Merging of CSV tables

- Prior to the upload to MCRA, the CSV tables need to be merged to one excel table
 - Also, other formatting steps need to be conducted
 - Not very hard, but time-consuming
- Prepared excel table is provided on USB Stick
- Instructions for merging and formating in back-up slides



Please log in as done in
the previous trainings

MCRA 8.2

MCRA stands for **Monte Carlo Risk Assessment**.

MCRA is a web-based system for probabilistic exposure and risk assessment of chemicals in the diet.

The MCRA system brings together statistical models, shared data and data uploaded by the user.

MCRA 8 also provides **Cumulative Exposure Assessment** for chemicals grouped in a Cumulative Assessment Group for which a single health effect is considered relevant.

Optionally exposure from other routes can be added in an **Aggregate Exposure Assessment**.

MCRA 8 was developed in [EU project ACROPOLIS](#) and is further developed in actions for EFSA and in [EU project EuroMix](#)

[Publications and reports using MCRA](#)

Login

Username

Password

[Go to registration](#)

LOGIN

Create new project

project

MCRA

Monte Carlo Risk Assessment

General options

[Open an existing project](#)

[Create a new project](#)

[Open file manager](#)

New Project

X

Enter Name, Tag(s) and Description for your new project. Choose a scenario (default is exposure) and type of exposure (Acute or Chronic). A single compound analysis is default or check the boxes for other options.

Name

EuroToxBPA

Tags

Description

Click to edit..

Exposure type

Acute

Cumulative exposure

Hide advanced settings

Assessment type

Exposure

Aggregate exposure

Use focal commodity

Submit



Data selection

data

Data [?]

✓ **Foods*** [clear](#)

Selected file: Foods MCRA_EuroTox.xlsx [change](#)

✓ **Compounds*** [clear](#)

Selected file: compoundsBPA_EuroTox.xlsx [change](#)

✓ **Consumptions*** [clear](#)

Selected file: consumptions_EuroTox_v2.xlsx [change](#)

✓ **Concentrations*** [clear](#)

Selected file: concentrationsBPA_EuroTox.xlsx [change](#)

✓ **Non-dietary*** [clear](#)

Selected file: MCRATablePCPs.xlsx [change](#)

[Show advanced settings](#)

File manager



File Name	Modification Date
adultResident_NDExpCombined_s5pc.mdb	20/08/2018 01:58 PM
compoundsBPA_EuroTox.xlsx	20/08/2018 01:56 PM
concentrationsBPA_EuroTox.xlsx	20/08/2018 01:56 PM
consumptions_EuroTox_v2.xlsx	20/08/2018 01:57 PM
Foods MCRA_EuroTox.xlsx	20/08/2018 01:57 PM
MCRATablePCPs.xlsx	20/08/2018 01:57 PM
TrainingEuromix - all MoA.mdb	20/08/2018 01:57 PM
TrainingEuromix - Concentrations all MoA.mdb	20/08/2018 01:57 PM
TrainingEuromixNonDietarydermad0.1.mdb	20/08/2018 02:04 PM

Clear All

Save/Next step >>



select

Select [?]

Food survey

Compounds

Conversion

Population Subsets

Food Subsets

Sample Subsets

Select a food survey from the list.

Food consumption survey



EuroTox_course



Save/Next step >>



Selection panel

select

Select [?]

Compounds Conversion Population Subsets Food Subsets Sample Subsets

Select a compound from the list.

Compound



Bisphenol A (Total)



Save/Next step >>



Conversion Population Subsets Food Subsets Sample Subsets

Foods as eaten (table FoodConsumption) are converted to foods as measured (table ConcentrationPersample or table TabulatedConcentration). A 7- step recursive food code conversion algorithm is applied (click Help for more information).

[Hide advanced settings](#)

Include foods with only non-detect measurements

Include compounds with only non-detect measurements

Step 2: allow conversion 'using processing' info

Step 3a, 3b: allow conversion using 'food translation' info

Step 3c: allow conversion using 'read across' info

Step 4: allow marketshares not summing to 100%

Step 5: allow conversion to supertypes

Step 6: allow conversion using default processing factors

Step 7: allow maximum residue limit data

Untick everything
(we are not using
processing infos or food
translations)

select

Select [?]

Conversion

Population Subsets

Food Subsets

Sample Subsets

Select specific groups of individuals based on available cofactors (select levels) and covariates (select minimum and maximum value).

Use population subsets

[Show advanced settings](#)

Save/Next step >>



select

Select [?]

Conversion

Population Subsets

Food Subsets

Sample Subsets

Specify subsets of foods as eaten (in table FoodConsumption) and foods as measured (in table ConcentrationPerSample or table TabulatedConcentration). The two lists will adapt to each other, e.g. selecting only food as measured Apple will delete food as eaten Milk from the food as eaten list (no Apple in Milk). Note: the first time execution may take a long time, since a food conversion is performed.

**Use food selection to restrict population
(consumption-days or consumers only)**

Use food selection to restrict foods

Save/Next step >>



Selection panel

select

Select [?]

Conversion Population Subsets Food Subsets **Sample Subsets**

Select subsets of the analysed samples to be included in the exposure assessment, regarding the country of origin of the samples (location) and year in which the samples were analysed.

Use sample subsets

Save/Next step >>



Model [?]

Exposures Concentrations Unit-variability Aggregate Monte-Carlo Uncertainty Output

Choose the exposure model tier or configure a custom exposure model. To model chronic exposure five models are available: OIM, BBN, LNN0, LNN and ISUF (click Help for explanation). Food consumption data with only 1 day per individual can be included in a chronic exposure assessment by filling in a value for dispersion and variance ratio For acute exposure two models (BBN, LNN0) are available to model the simulated exposures as a function of covariates.

Dietary exposure calculation tier

Dietary intake method

[Hide advanced settings](#)

Covariate modelling

Impute exposure distributions

Save/Next step >>



Model [?]

Exposures Concentrations Unit-variability Aggregate Monte-Carlo Uncertainty Output

Concentration data can be sampled directly from the data (empirical model) or from parametric models. Concentrations < LOR (Limit Of Reporting) (non-detects) can be co-modelled (censored models) or one can specify a non-detects handling method for imputation. Agricultural use data can be used to impose true zeroes for all or part of the non-detects. Effects of processing on concentrations can be specified using processing factors

Concentration model

Default concentration model 

Include MRL fallback model

Non-detects replacement

• Factor f (f x LOR)

Consumptions on the same day come from the same sample

[Show advanced settings](#)

Show concentration models

Save/Next step >>



model

Model [?]

Exposures Concentrations **Unit-variability** Aggregate Monte-Carlo Uncertainty Output

If concentrations are measured in composite samples part of the variability that exists between individual units is masked. MCRA can model unit variability by sampling from a Beta, Bernoulli or Lognormal distribution.

Unit variability model

No unit-variability ▼

Save/Next step >>



model

Model [?]

Exposures Concentrations Unit-variability **Aggregate** Monte-Carlo Uncertainty Output

To aggregate dietary and non-dietary exposures, the non-dietary exposures can be matched to specific individuals in the food survey or they can be randomly assigned. If matching is enabled, any 'idIndividuals' in the 'NonDietaryExposures' table that do not correspond to individuals in the food survey will be ignored. For the unmatched case, a correlation between 'idIndividuals' in different surveys can be applied or not. The aggregate exposure is calculated as an absorbed (internal) dose. Dietary exposures are multiplied by the oral absorption factor to determine the internal dose.

Match to specific dietary survey individuals

Apply correlation between identical individuals (based on id) in different nondietary surveys

Oral absorption factor for dietary exposure

Save/Next step >>



Modeling panel

model

Model [?]

Exposures Concentrations Unit-variability Aggregate **Monte-Carlo** Uncertainty Output

Settings for the Monte Carlo simulation

Number of Monte Carlo simulations

Seed for pseudo-random number generator

[Show advanced settings](#)

Save/Next step >>



Model [?]

Exposures Concentrations Unit-variability Aggregate Monte-Carlo **Uncertainty** Output

Uncertainty is quantified by performing repeated analyses using resampled data. Results are displayed in the form of approximate confidence intervals. Warning: computation time may be substantially longer.

Perform uncertainty analysis

Number of iterations per resampled set

Number of resample cycles

Resample concentrations

• Parametric uncertainty

Resample individuals

Resample nondietary exposures.

[Show advanced settings](#)

Save/Next step >>



Exposures Concentrations Unit-variability Aggregate Monte-Carlo Uncertainty **Output**

Specify details of output that will be generated

Show percentiles for

Percentage for upper tail

Show % of population below level(s)

• Exposure levels

• Exposure levels are

Include drill-down on 9 individuals around specified percentile. ←

[Hide advanced settings](#)

Summarize simulated data ←

Store simulated individual day exposures ←

Percentage for drilldown

Number of levels of covariable to predict exposure

Predict exposure at extra covariable levels

Lower percentage (default interquartile 25%)

Upper percentage (default interquartile 75%)



Data

Foods:	Foods MCRA_EuroTox.xlsx
Compounds:	compoundsBPA_EuroTox.xlsx
Consumptions:	consumptions_EuroTox.xlsx
Concentrations:	concentrationsBPA_EuroTox.xlsx
Non-dietary:	MCRAtablePCPs.xlsx

Select

Food consumption survey:	EuroTox_course
--------------------------	----------------

Model

Exposure calculation tier:	Custom
Dietary exposures method:	Distribution estimates
Concentration model:	Non-Detect Spike LogNormal, nondetects set to zero. fixed processing factors.
Aggregate exposure:	oral absorption factor for dietary exposure = 1
Number of Monte Carlo simulations:	100000
Uncertainty analysis:	No

Run

Run

Click and wait until run is completed

Output panel

output


Output ?

Selection (0):

Output	Completed	Description	Select
short	14-8-2018	<input type="text" value="Edit description..."/>	<input type="checkbox"/>
detailed	12:16:56		<input type="checkbox"/>
conversion			<input type="checkbox"/>



EuroToxBPA

 Download

MCRA version	8.2.20 (build date: 6/4/2018 9:27:17 AM)
Output creation date	8/14/2018 12:16:56 PM
Execution time	0:00:56


- Input settings/model parameters
- Conversion of food codes
- Input data
- Acute exposure assessment

- Check settings & parameters
- Food as eaten vs. food as measured
- Consumptions, concentrations, ND data
- Exposure assessment results



Results – ND data

Non-dietary data

 Download



Non-dietary survey	Compound name	Compound code	Case?	Total individuals	Mean dermal exposure (ng/day)	Dermal absorption factor	Mean oral non-dietary exposure (ng/day)	Oral absorption factor	Mean inhalation exposure (ng/day)	Inhalation absorption factor
1	Bisphenol A (Total)	RF-00000482-ORG	Unmatched	5,000	100	0.2	0.484	1	0	1
2	Bisphenol A (Total)	RF-00000482-ORG	Unmatched	5,000	29	0.2	0.0486	1	0	1

Individuals exposed to nondietary sources (unmatched) are restricted according to the covariates settings below:



Code	Description	Covariate	PropertyType	Level	Minimum value	Maximum value
1	PACEM output	Gender	Cofactor	female	0	0
2	PACEM output	Gender	Cofactor	male	0	0




Code	Description	Percentage zeros (%)	Number of exposure sets
1	PACEM output	0	5,000
2	PACEM output	0	5,000



Results – exposure options

+ Dietary exposure by food-compound

- Dietary exposure by food

 Download

+ Food as measured total distribution

+ Food as measured upper tail


+ Food as eaten total distribution

+ Food as eaten upper tail

Same information if only one chemical is regarded

Same information if no recipes or food translations are used

- Non-dietary exposure by route

 Download

+ NonDietary exposure total distribution by route and compound


+ NonDietary exposure total distribution by route

+ NonDietary exposure upper tail by route and compound


+ NonDietary exposure upper tail by route

Results – dietary exposure

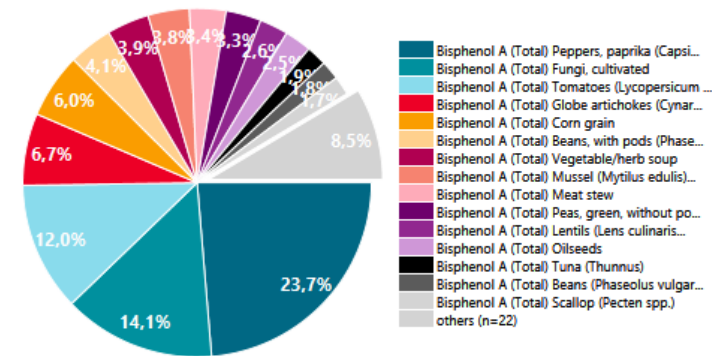
▣ Dietary exposure by food-compound

 Download

▣ Risk drivers total distribution

 Download

Contribution to total exposure distribution for foods as measured x compounds (MSCC)



Compound name	Food name	Contribution (%)	individual days with exposure	Mean exposure all individual days (µg/kg bw/day)	Median for all individual days (µg/kg bw/day)	p25 for all individual days (µg/kg bw/day)	p75 for all individual days (µg/kg bw/day)	Percentage individual days with exposure (%)	Mean exposure for individual days exposure > 0 (µg/kg bw/day)	Median (µg/kg bw/day)	p25 (µg/kg bw/day)	p75 (µg/kg bw/day)
Bisphenol A (Total)	Peppers, paprika (Capsicum annuum, var. grossum and var. longum)	23.7	17,781	0.00028	0	0	0	17.8	0.00157	0.00107	0.000588	0.00191
Bisphenol A (Total)	Fungi, cultivated	14.1	13,271	0.000167	0	0	0	13.3	0.00126	0.000321	0.000104	0.000993
Bisphenol A (Total)	Tomatoes (Lycopersicon esculentum)	12.0	15,716	0.000141	0	0	0	15.7	0.0009	0.000383	0.000161	0.000927
Bisphenol A (Total)	Globe artichokes (Cynara scolymus)	6.7	13,788	7.9E-05	0	0	0	13.8	0.000573	0.000298	0.000133	0.000643

Results are for illustration purposes - No risk assessment

EuroTox CEC – 2 Sept, 2018

This project is funded by the Horizon 2020 Framework Programme of the European Union

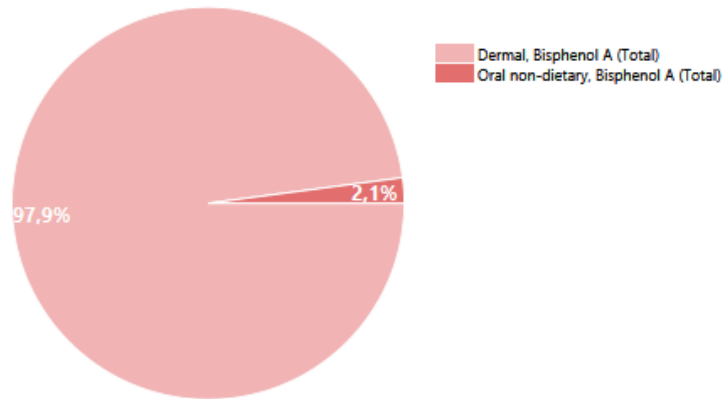


Results – non-dietary exposure

NonDietary exposure total distribution by route and compound

 Download

Contribution to the total exposure distribution by route x compound



Exposure Route	Compound name	Compound code	Contribution	individual days with exposure	Mean exposure all individual days (µg/kg bw/day)	Median all individual days (µg/kg bw/day)	p25 all individual days (µg/kg bw/day)	p75 all individual days (µg/kg bw/day)	Percentage individual days with exposure > 0	Mean individual days exposure > 0 (µg/kg bw/day)	Median individual days exposure > 0 (µg/kg bw/day)	p25 individual days exposure > 0 (µg/kg bw/day)	p75 individual days exposure > 0 (µg/kg bw/day)	RPF ?
Dermal	Bisphenol A (Total)	RF-00000482-ORG	97.9	57,268	0.000191	1.65E-06	0	0.000123	57.3	0.000334	9.35E-05	1.9E-05	0.000255	1
Oral non-dietary	Bisphenol A (Total)	RF-00000482-ORG	2.1	28,446	4.08E-06	0	0	3.08E-06	28.4	1.43E-05	8.54E-06	4.5E-06	1.7E-05	1


Results are for illustration purposes - No risk assessment

EuroTox CEC – 2 Sept, 2018




Results – aggregate exposure

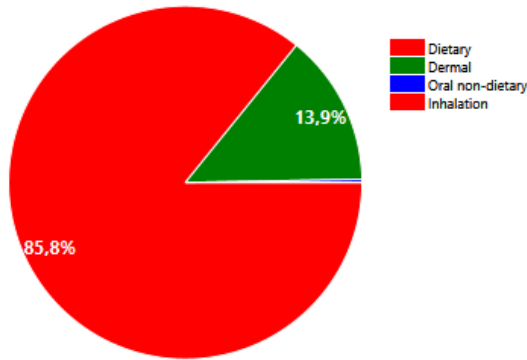
Aggregate exposure by route

 Download

Exposure total distribution by route

 Download

Contribution to the total exposure distribution by route



Exposure Route	Contribution	individual days with exposure	Mean exposure all individual days (µg/kg bw/day)	Median all individual days (µg/kg bw/day)	p25 all individual days (µg/kg bw/day)	p75 all individual days (µg/kg bw/day)	Percentage individual days with exposure > 0	Mean exposure individual days exposure > 0 (µg/kg bw/day)	Median individual days exposure > 0 (µg/kg bw/day)	p25 individual days exposure > 0 (µg/kg bw/day)	p75 individual days exposure > 0 (µg/kg bw/day)
Dietary	85.8	99,911	0.00118	0.000562	0.00029	0.00121	99.9	0.00118	0.000563	0.000291	0.00121
Dermal	13.9	57,268	0.000191	1.65E-06	0	0.000123	57.3	0.000334	9.35E-05	1.9E-05	0.000255
Oral non-dietary	0.3	28,446	4.08E-06	0	0	3.08E-06	28.4	1.43E-05	8.54E-06	4.5E-06	1.7E-05
Inhalation	0.0	0	-	0	0	0	0.0	-	0	0	0

Results are for illustration purposes - No risk assessment

EuroTox CEC – 2 Sept, 2018



Results – exposure distributions

Exposure distribution

Download

Dietary

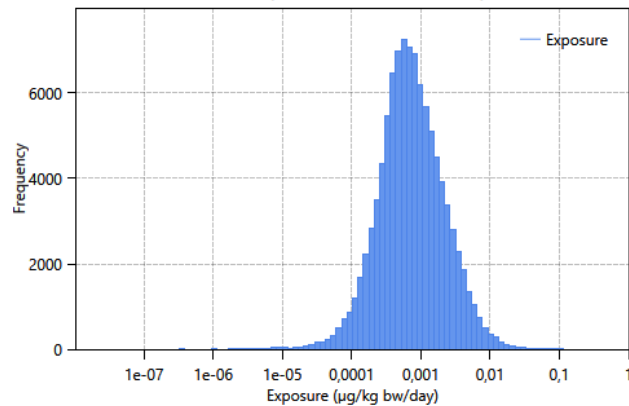
Non-dietary

Aggregate

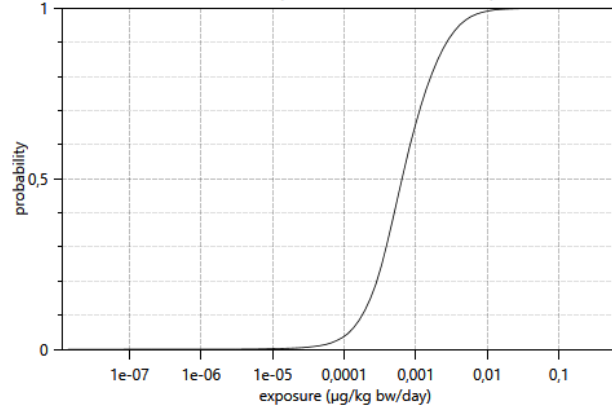
Total

Download

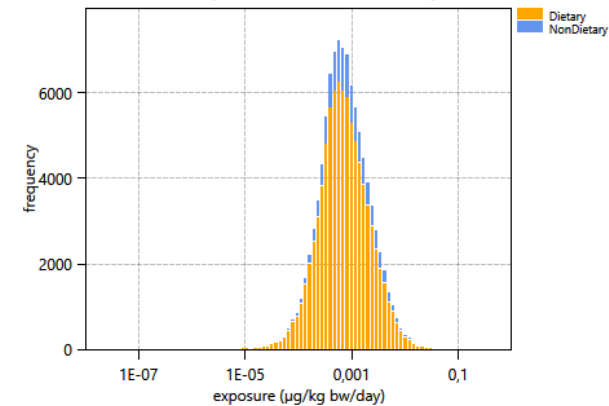
Transformed exposure distribution (100.0% positives)



Cumulative acute exposure distribution (100.0% positives)



Transformed exposure distribution (100.0 % positives)



Other analysis options:

- Percentile tables
- Detailed look at individual exposures in drilldown
- Uncertainty analysis can be added

Results are for illustration purposes - No risk assessment

EuroTox CEC – 2 Sept, 2018



Acknowledgements



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Christiaan Delmaar
Bas Bokkers



Safety and
Environmental
Technology Group

Thank you for your attention and participation!

Are there questions, comments etc.?

EuroTox CEC – 2 Sept, 2018



EuroMix

EuroMix participants

22 beneficiaries from 16 countries linked to international organisations including WHO, FAO and EFSA.
EuroMix is coordinated by RIVM.



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Back-up



PACEM – exposure calculation

Dose D_{ij} on day j

$$D_{ij} = \frac{1}{BW_i} \sum_k n_{ijk} * A_{ik} * wf_k * ef_k$$

BW_i : body weight of i
 n_{ijk} : number of uses
of k by i on j



Product k

A_{ik} : amount of k used by i
 wf_k : concentration of
substance in k

Individual i

ef_k : fraction of substance from k
absorbed by i

Workflow of PACEM Shiny

Assessment definition

- Start new assessment or select existing
- Select survey and exposure metric

Data input

- Fill concentration table
- Fill table for exposure fractions (systemic exposure) or retention factors (dermal load)

Define model scope

- Specify number of days, female and male persons

Analysis options

- Select exposure routes, exposure measure (acute or chronic), population and/or product subsets and percentiles to be displayed
- Option to provide results suitable for use in the MCRA model

Results

- Percentile table, histograms, cumulative density functions, table with detailed simulation results

MCRA inputs

- Tables for further use in the MCRA model can be exported
- Stratification by gender possible



Concentration data

Product	DF [%]	Distribution	Mean [ng/g]	SD	Min	Max	Use for
Shampoo	20.0	Uniform			18.1	60.4	Shampoo & conditioner
Face cleanser	11.1	TruncLognorm	60.6	30.2	18.1	121	Cleansing lotion
Bath gel	4.8	Uniform			18.1	60.4	Shower gel, bathing foam, bathing oil
Sunscreen	41.7	TruncLognorm	95.3	55.8	18.1	207	Sunscreen, after-sun cream, Bronzing cream
Body lotion	25.0	Uniform			18.1	60.4	Body lotion
Lipstick	100	Uniform			18.1	60.4	Lipstick, lipbalm
Hand lotion	52.9	Uniform			18.1	60.4	Hand cream
Face mask	72.7	TruncLognorm	107	46.9	18.1	200	Aftershave balsam, Face cream day & night

DF = detection frequency



Upload input tables

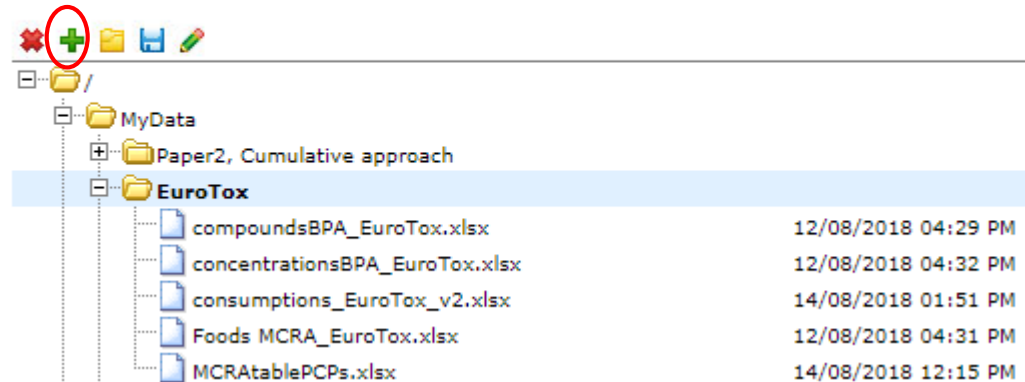
project

MCRA
Monte Carlo Risk Assessment

General options

- [Open an existing project](#)
- [Create a new project](#)
- [Open file manager](#)

File manager



The file manager interface shows a tree view of folders and files. The 'EuroTox' folder is selected and highlighted in blue. It contains five files:

File Name	Timestamp
compoundsBPA_EuroTox.xlsx	12/08/2018 04:29 PM
concentrationsBPA_EuroTox.xlsx	12/08/2018 04:32 PM
consumptions_EuroTox_v2.xlsx	14/08/2018 01:51 PM
Foods MCRA_EuroTox.xlsx	12/08/2018 04:31 PM
MCRAtablePCPs.xlsx	14/08/2018 12:15 PM

If not already available, add all five data files from the folder «Datasets MCRA» (USB Stick) to the folder «MyData»



Merge CSV tables (I)

- Open all tables
- Save the largest table ('saveMCRAtable', if not renamed) as excel file and use as basis for adding the other tables

In the excel file:

- Rename the existing sheet to '***NonDietaryExposures***'
- Add three empty sheet and name them '***NonDietarySurveys***', '***NonDietarySurveyProperties***', and '***NonDietaryAbsorptionFactors***'

NonDietaryExposures	NonDietarySurveys	NonDietarySurveyProperties	NonDietaryAbsorptionFactors
---------------------	-------------------	----------------------------	------------------------------------

- Copy the content of the three remaining CSV tables into the empty sheets



Merge CSV tables (II)

	A	B	C	D	E	F	G	H	I
1	idIndividual,"idNonDietarySurvey","idSubstance","Dermal","Oral","Inhalation"								
2	PACEM_1,2,"RF-00000482-ORG",0.0335277982694903,0.301750184425412,0								
3	PACEM_2,2,"RF-00000482-ORG",0.0747236495882002,0.672512846293802,0								
4	PACEM_3,2,"RF-00000482-ORG",1.15484182625043,0,0								
5	PACEM_4,2,"RF-00000482-ORG",17.0508004139567,1.44886136668451,0								
6	PACEM_5,2,"RF-00000482-ORG",17.9244460996482,0,0								

Navigation: NonDietaryExposures | NonDietarySurveys | NonDietarySurveyProperties

	A	B	C	D	E	F	G	H	I
1	idNonDietarySurvey,"Description","NonDietaryIntakeUnit","PercentageZeros"								
2	1,"PACEM output 2018-07-25","nanogram/day",0								
3	2,"PACEM output 2018-07-25","nanogram/day",0								

Navigation: NonDietaryExposures | NonDietarySurveys | NonDietarySurveyProperties

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	IndividualPropertyName,"idNonDietarySurvey","IndividualPropertyTextValue","IndividualPropertyDoubleValueMin","IndividualPropertyDoubleValueMax"														
2	Gender,1,"female",0,0														
3	Gender,2,"male",0,0														

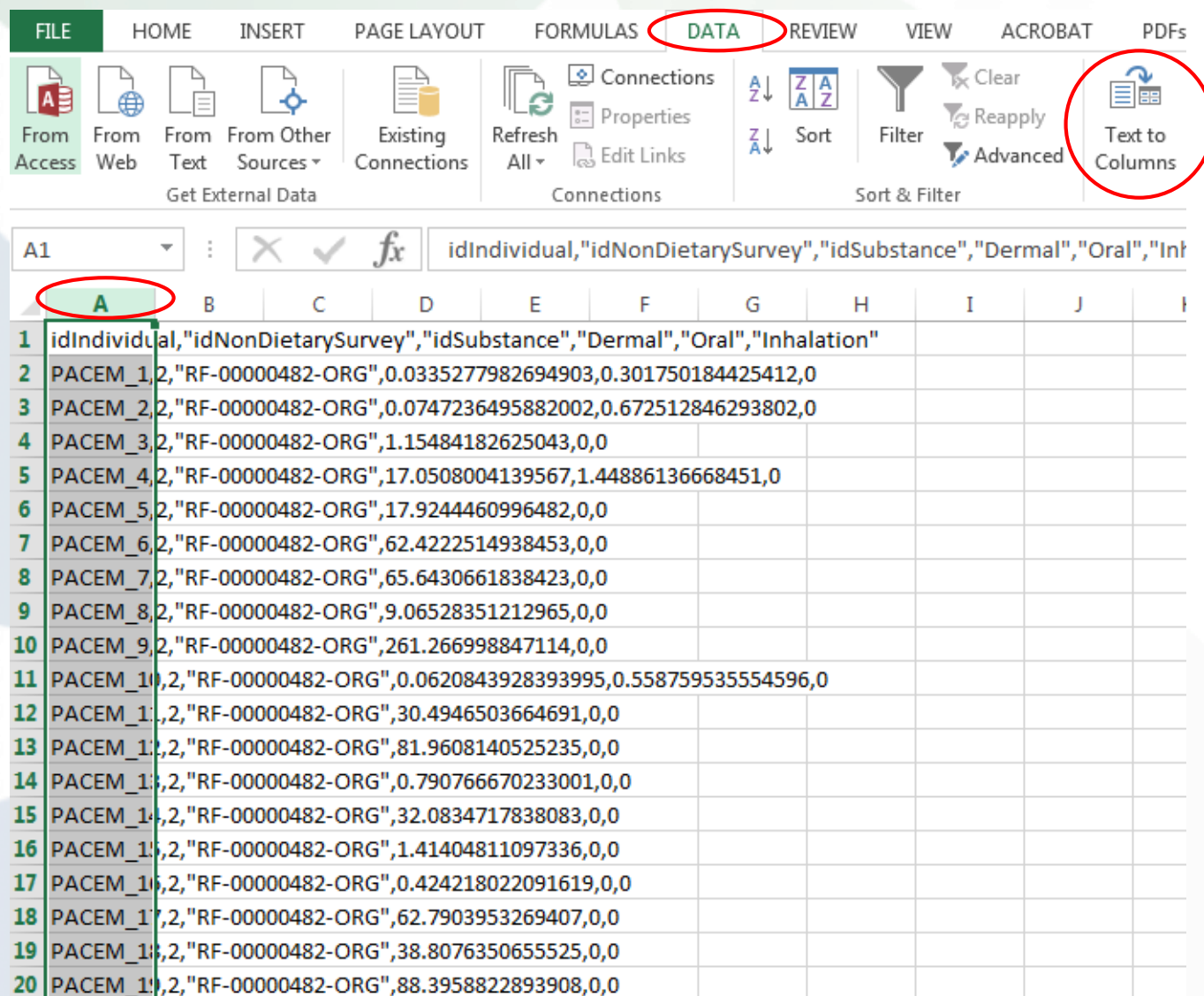
Navigation: NonDietaryExposures | NonDietarySurveys | NonDietarySurveyProperties

	A	B	C	D	E	F	G	H	I	J	K	L
1	idNonDietarySurvey,"idCompound","DermalAbsorptionFactor","OralAbsorptionFactor","InhalationAbsorptionFactor"											
2	1,"RF-00000482-ORG",0.2,1,1											
3	2,"RF-00000482-ORG",0.2,1,1											

Navigation: NonDietaryExposures | NonDietarySurveys | NonDietarySurveyProperties | NonDietaryAbsorptionFactors



Split text to columns (I)



Excel ribbon: FILE, HOME, INSERT, PAGE LAYOUT, FORMULAS, DATA, REVIEW, VIEW, ACROBAT, PDFs

Buttons: From Access, From Web, From Text, From Other Sources, Existing Connections, Refresh All, Connections, Properties, Edit Links, Sort, Filter, Clear, Reapply, Advanced, Text to Columns

Formula bar: A1 : \times \checkmark fx idIndividual,"idNonDietarySurvey", "idSubstance", "Dermal", "Oral", "Inf

A	B	C	D	E	F	G	H	I	J	K
1	idIndividual,"idNonDietarySurvey", "idSubstance", "Dermal", "Oral", "Inhalation"									
2	PACEM_1	2,"RF-00000482-ORG"	0.0335277982694903	0.301750184425412	0					
3	PACEM_2	2,"RF-00000482-ORG"	0.0747236495882002	0.672512846293802	0					
4	PACEM_3	2,"RF-00000482-ORG"	1.15484182625043	0,0						
5	PACEM_4	2,"RF-00000482-ORG"	17.0508004139567	1.44886136668451	0					
6	PACEM_5	2,"RF-00000482-ORG"	17.9244460996482	0,0						
7	PACEM_6	2,"RF-00000482-ORG"	62.4222514938453	0,0						
8	PACEM_7	2,"RF-00000482-ORG"	65.6430661838423	0,0						
9	PACEM_8	2,"RF-00000482-ORG"	9.06528351212965	0,0						
10	PACEM_9	2,"RF-00000482-ORG"	261.266998847114	0,0						
11	PACEM_10	2,"RF-00000482-ORG"	0.0620843928393995	0.558759535554596	0					
12	PACEM_11	2,"RF-00000482-ORG"	30.4946503664691	0,0						
13	PACEM_12	2,"RF-00000482-ORG"	81.9608140525235	0,0						
14	PACEM_13	2,"RF-00000482-ORG"	0.790766670233001	0,0						
15	PACEM_14	2,"RF-00000482-ORG"	32.0834717838083	0,0						
16	PACEM_15	2,"RF-00000482-ORG"	1.41404811097336	0,0						
17	PACEM_16	2,"RF-00000482-ORG"	0.424218022091619	0,0						
18	PACEM_17	2,"RF-00000482-ORG"	62.7903953269407	0,0						
19	PACEM_18	2,"RF-00000482-ORG"	38.8076350655525	0,0						
20	PACEM_19	2,"RF-00000482-ORG"	88.3958822893908	0,0						



Split text to columns (II)

Convert Text to Columns Wizard - Step 1 of 3

The Text Wizard has determined that your data is Delimited.
If this is correct, choose Next, or choose the data type that best describes your data.

Original data type

Choose the file type that best describes your data:

Delimited Characters such as commas or tabs separate each field.
 Fixed width Fields are aligned in columns with spaces between each field.

Preview of selected data:

1	idIndividual	"idNonDietarySurvey"	"idSubstance"	"Dermal"	"Oral"
2	PACEM_1_2	"RF-00000482-ORG"	0.0335277982694903	0.30175018442541	
3	PACEM_2_2	"RF-00000482-ORG"	0.0747236495882002	0.67251284629380	
4	PACEM_3_2	"RF-00000482-ORG"	1.15484182625043	0,0	
5	PACEM_4_2	"RF-00000482-ORG"	17.0508004139567	1.44886136668451	0

Cancel < Back Next > Finish

Convert Text to Columns Wizard - Step 2 of 3

This screen lets you set the delimiters your data contains. You can see how your text is affected in the preview below.

Delimiters

Tab
 Semicolon
 Comma
 Space
 Other:

Treat consecutive delimiters as one

Text qualifier:

Data preview

idIndividual	idNonDietarySurvey	idSubstance	Dermal
PACEM_1	2	RF-00000482-ORG	0.033527798269490
PACEM_2	2	RF-00000482-ORG	0.074723649588200
PACEM_3	2	RF-00000482-ORG	1.15484182625043
PACEM_4	2	RF-00000482-ORG	17.0508004139567

Cancel < Back Next > Finish

Convert Text to Columns Wizard - Step 3 of 3

This screen lets you select each column and set the Data Format.

Column data format

General
 Text
 Date: DMY
 Do not import column (skip)

'General' converts numeric values to numbers, date values to dates, and all remaining values to text.

Advanced...

Destination: SAS1

Data preview

General	General	General	General
idIndividual	idNonDietarySurvey	idSubstance	Dermal
PACEM_1	2	RF-00000482-ORG	0.033527798269490
PACEM_2	2	RF-00000482-ORG	0.074723649588200
PACEM_3	2	RF-00000482-ORG	1.15484182625043
PACEM_4	2	RF-00000482-ORG	17.0508004139567

Cancel < Back Next > Finish



Format columns (II)

Table	Column	Type
NonDietary Exposures	idIndividual	Text
	idNonDietarySurvey	
	idSubstance	
	Dermal	
	Oral	
	Inhalation	Number (5 decimal places)
NonDietary SurveyProperties	IndividualPropertyName	Text
	idNonDietarySurvey	
	IndividualPropertyTextValue	
	IndividualPropertyDoubleValueMin	
	IndividualPropertyDoubleValueMax	
NonDietary Surveys	idNonDietarySurvey	Text
	Description	
	NonDietaryIntakeUnit	
	PercentageZeros	
		Number*
NonDietary Absorption Factors	idNonDietarySurvey	Text
	idCompound	
	DermalAbsorptionFactor	
	OralAbsorptionFactor	
	InhalationAbsorptionFactor	
		Number

*by default entries with zero exposures are included in the dataset, so that the percentage of zeroes is 0

