LIMS SHINY Application

v.0.1.0

A shiny application for creating ImproRisk occurrence templates

Description and User Manual

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App build specification

The app can be found on https://sglcy.shinyapps.io/lims/

It hosted on the https://www.shinyapps.io server managed by Rstudio [https://rstudio.com]

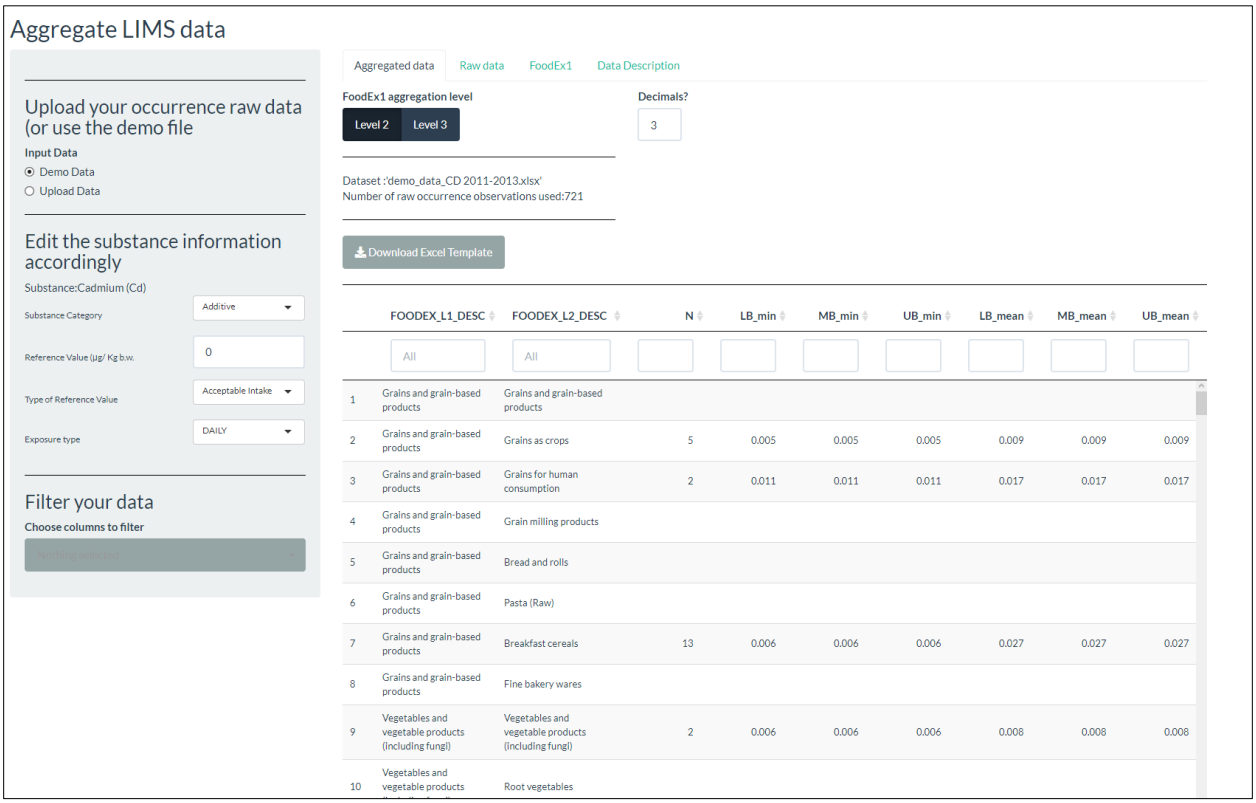
The app is built as a shiny application [https://shiny.rstudio.com] and it runs on the R statistical programming language [https://www.r-project.org]

The app is built on the R v.3.6.3 and the Shiny package v.1.5.0

On load

When the app loads, the initial screen is as seen in Figure 1.

Figure 1 Initial screen when app loads

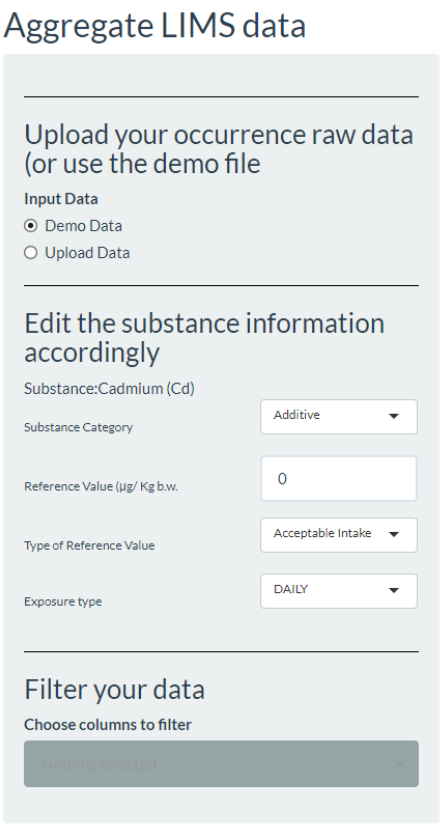


	FOODEX_L1_DESC	FOODEX_L2_DESC	N	LB_min	MB_min	UB_min	LB_mean	MB_mean	UB_mean
	All	All							
1	Grains and grain-based products	Grains and grain-based products							
2	Grains and grain-based products	Grains as crops	5	0.005	0.005	0.005	0.009	0.009	0.009
3	Grains and grain-based products	Grains for human consumption	2	0.011	0.011	0.011	0.017	0.017	0.017
4	Grains and grain-based products	Grain milling products							
5	Grains and grain-based products	Bread and rolls							
6	Grains and grain-based products	Pasta (Raw)							
7	Grains and grain-based products	Breakfast cereals	13	0.006	0.006	0.006	0.027	0.027	0.027
8	Grains and grain-based products	Fine bakery wares							
9	Vegetables and vegetable products (including fungi)	Vegetables and vegetable products (including fungi)	2	0.006	0.006	0.006	0.008	0.008	0.008
10	Vegetables and vegetable products	Root vegetables							

Side bar panel

On the left, there is a grey shaded side-bar panel (Figure 2) with three sections:

Figure 2 App Side Bar Panel



Section: Upload occurrence data or use demo file

Here, the user can

a) Use the demo data already installed. These are data for demonstration purposes

b) Upload a dataset to repeat the analysis

Section: Edit the Substance Information

After, the user uploads their own set of data, she can fill in this information required by the ImproRisk. This information is not used in the aggregation rather the info is there to be placed in the final exported ImproRisk template for use within the ImproRisk.

The Substance name is automatically picked up from the data. In case the use uploads a dataset with information on more than one Substance, she can filter (keep) only the row data for a single substance using filters (see SECTION: Filter your data)

a) The substance category

The user can select between Additive", "Pesticide", "Veterinary Drug Residue", "Contaminant", or "Genotoxic-Carcinogen"

b) Reference value. The reference value for the substance. This should be numeric value greater than 0.

c) Type of reference value. Select one among "Acceptable Intake", "Tolerable Intake", "Provisional Maximum Tolerable Intake", or "Benchmark Dose Level (BMDL).

d) The exposure type. One of DAILY or WEEKLY

Section: Filter your data

Here the user can apply filtering to her data. Filtering in the sense of keeping what you want and reject what is not in our selections.

First, the user can select the columns where to filter on. On click, the user is given the list of column names the data contains to select (multiple selection is available) the columns to filter on. The filter has a build in smart search where options appear as the user types.(Figure 3)

The appropriate filters appear for the user to select particular values from the selected columns. (Figure 4)

Figure 3 UI - select columns to filter on

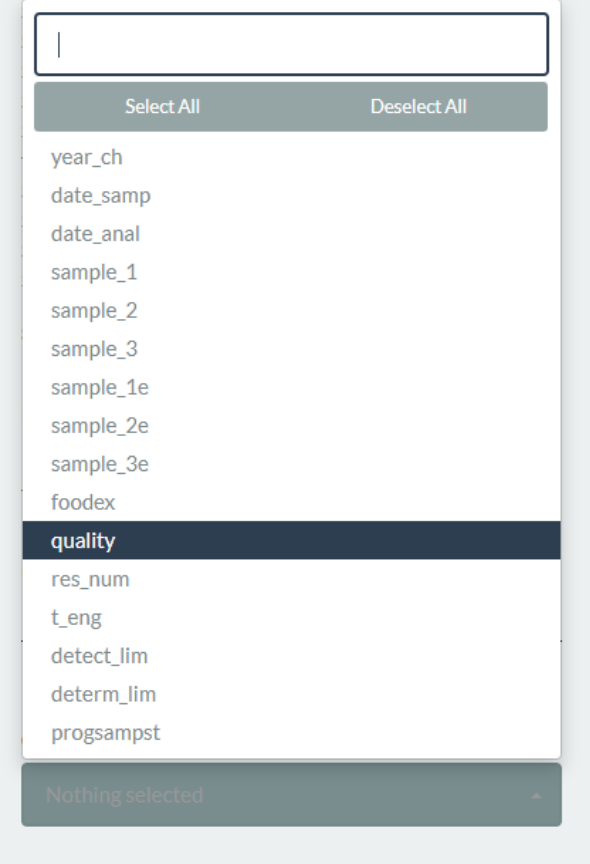
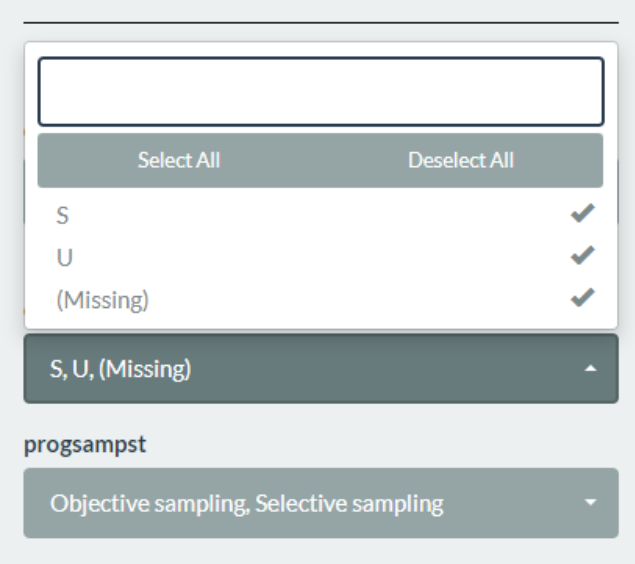


Figure 4 UI - Select the values from the columns to filter the data



Main panel

The main Panel (center of the screen) consists of 4 Tabs.

Aggregated data

Here, the user can view the aggregated data according the FoodEx1 categorization.

Additional options are

a) View the aggregation by Level 2 or Level 3

Note that the template is already prepared and contains both the Level 2 and Level 3 aggregations. This tab is for viewing purposes. Of course, if the user filters the dataset using the filters on the SIDE PANEL, the aggregation is recalculated.

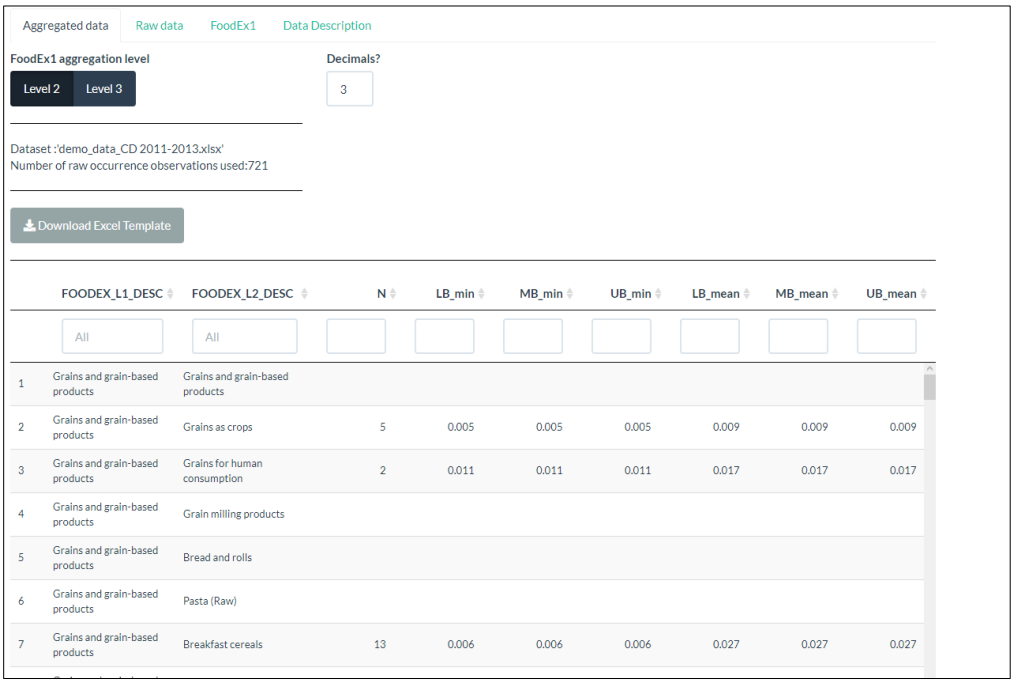
b) Set the number of decimals

Increase or decrease the decimal points in the aggregation values.

c) Download the template

Download the template in ".xlsx" format.

Figure 5 Aggregated Data TAB



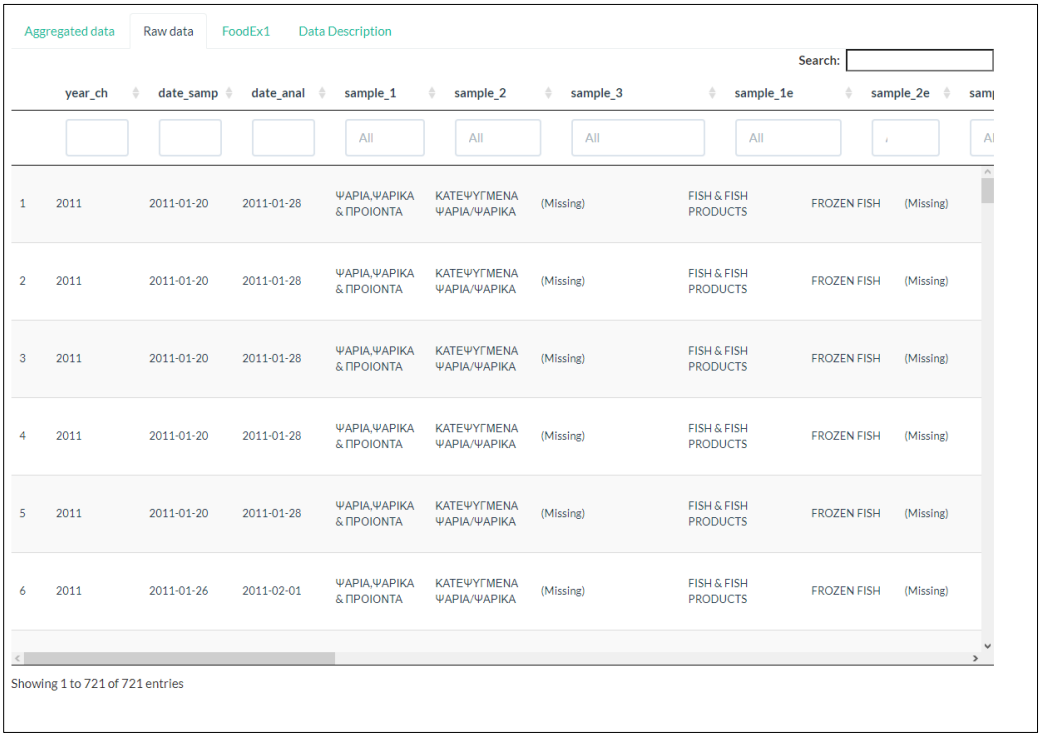
	FOODEX_L1_DESC	FOODEX_L2_DESC	N	LB_min	MB_min	UB_min	LB_mean	MB_mean	UB_mean
	All	All							
1	Grains and grain-based products	Grains and grain-based products							
2	Grains and grain-based products	Grains as crops	5	0.005	0.005	0.005	0.009	0.009	0.009
3	Grains and grain-based products	Grains for human consumption	2	0.011	0.011	0.011	0.017	0.017	0.017
4	Grains and grain-based products	Grain milling products							
5	Grains and grain-based products	Bread and rolls							
6	Grains and grain-based products	Pasta (Raw)							
7	Grains and grain-based products	Breakfast cereals	13	0.006	0.006	0.006	0.027	0.027	0.027

Raw Data

Here the user can inspect the raw data used in the calculations. These data are filtered according the user's filtering (if any) on the SIDE BAR Panel.

Note that using the table filters (top of the column names) does not influence the aggregation calculations. The table filters have n effect only on viewing the raw data.

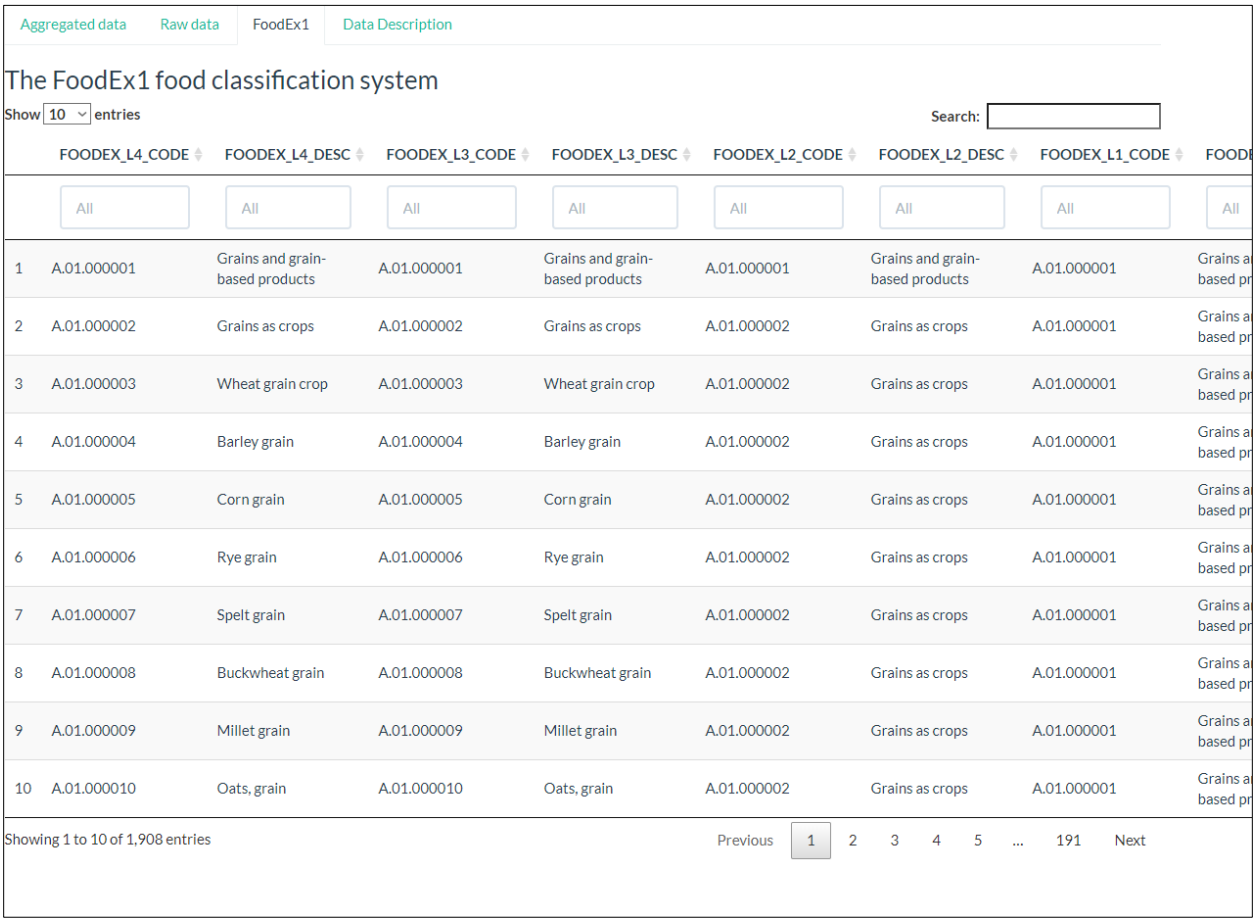
Figure 6 Raw Data TAB



FoodEx1

This Tab shows the FoodEx1 categorisation hierarchy. The table displays the FoodEx1 code and description on Level 4 thought Level 1.

Figure 7 FoodEx1 TAB



Aggregated data | Raw data | FoodEx1 | Data Description

The FoodEx1 food classification system

Show 10 entries Search:

	FOODEX_L4_CODE	FOODEX_L4_DESC	FOODEX_L3_CODE	FOODEX_L3_DESC	FOODEX_L2_CODE	FOODEX_L2_DESC	FOODEX_L1_CODE	FOODE
	All	All	All	All	All	All	All	All
1	A.01.000001	Grains and grain-based products	A.01.000001	Grains and grain-based products	A.01.000001	Grains and grain-based products	A.01.000001	Grains a based pr
2	A.01.000002	Grains as crops	A.01.000002	Grains as crops	A.01.000002	Grains as crops	A.01.000001	Grains a based pr
3	A.01.000003	Wheat grain crop	A.01.000003	Wheat grain crop	A.01.000002	Grains as crops	A.01.000001	Grains a based pr
4	A.01.000004	Barley grain	A.01.000004	Barley grain	A.01.000002	Grains as crops	A.01.000001	Grains a based pr
5	A.01.000005	Corn grain	A.01.000005	Corn grain	A.01.000002	Grains as crops	A.01.000001	Grains a based pr
6	A.01.000006	Rye grain	A.01.000006	Rye grain	A.01.000002	Grains as crops	A.01.000001	Grains a based pr
7	A.01.000007	Spelt grain	A.01.000007	Spelt grain	A.01.000002	Grains as crops	A.01.000001	Grains a based pr
8	A.01.000008	Buckwheat grain	A.01.000008	Buckwheat grain	A.01.000002	Grains as crops	A.01.000001	Grains a based pr
9	A.01.000009	Millet grain	A.01.000009	Millet grain	A.01.000002	Grains as crops	A.01.000001	Grains a based pr
10	A.01.000010	Oats, grain	A.01.000010	Oats, grain	A.01.000002	Grains as crops	A.01.000001	Grains a based pr

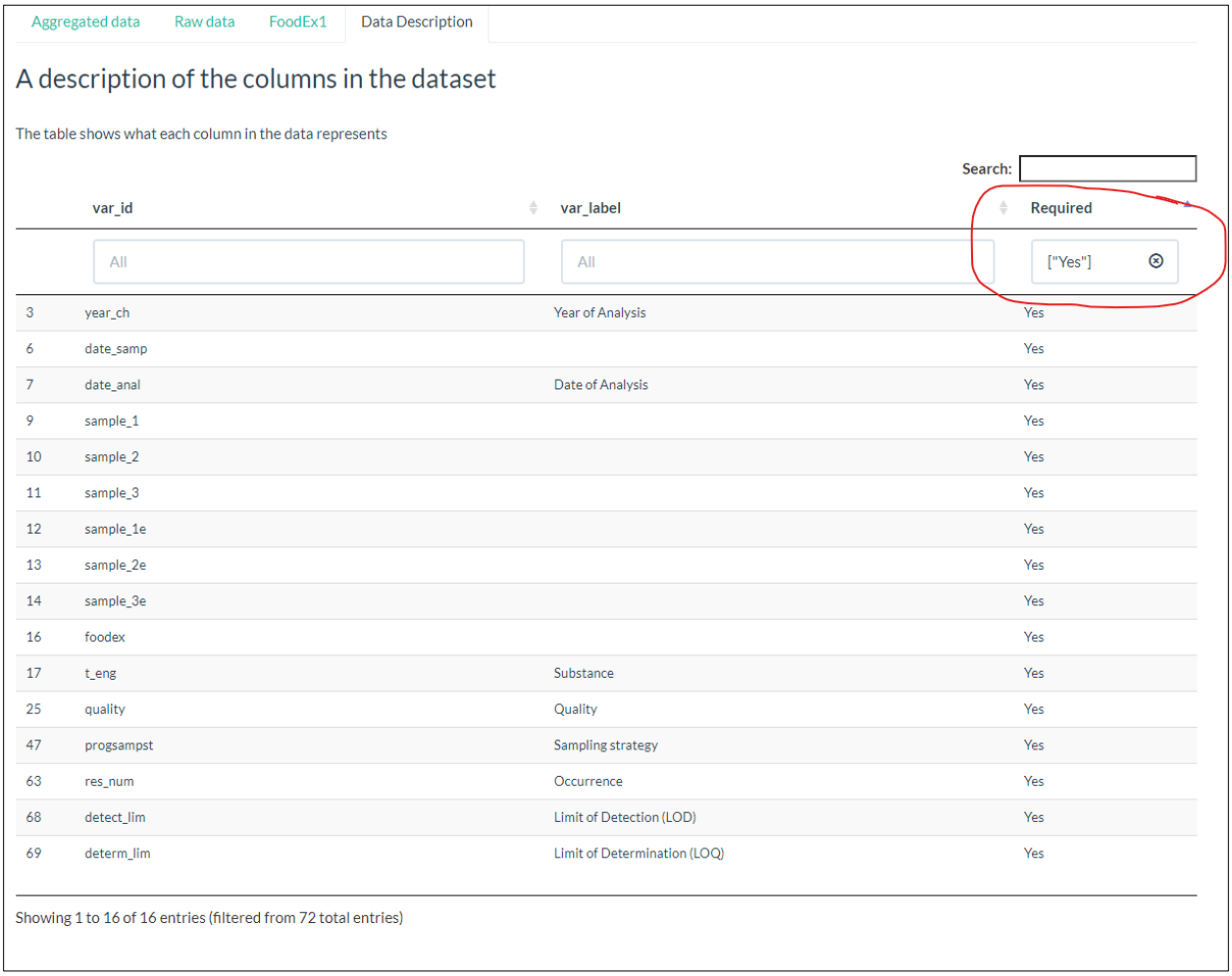
Showing 1 to 10 of 1,908 entries Previous 1 2 3 4 5 ... 191 Next

Data Description

This tab contains the data dictionary for the columns in the demo file that is built in the app.

It serves the purpose of showing the user, the necessary column names (and information they contain) for the app to calculate the aggregations. The user should upload data with at least the columns characterised as “Required” in the third column (Figure 8)

Figure 8 Data Description TAB



Download the excel template

In the “Aggregated Data” Tab, the user can download the excel template.

The excel template is an ”.xlsx” file with 2 worksheets (Level 2, Level 3) download in the default download directory of the user’s machine.(Figure 10)

Figure 9 Download Excel Template button

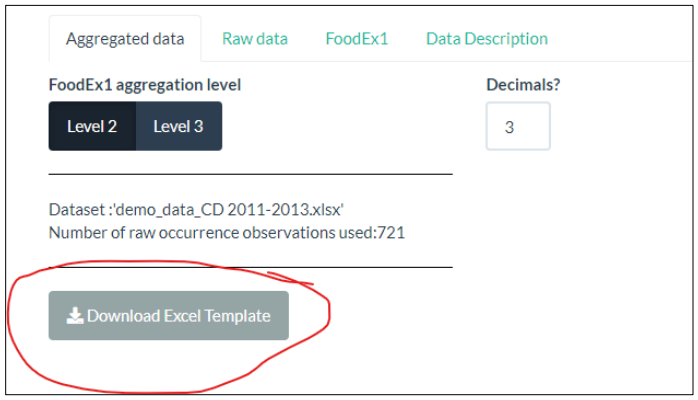
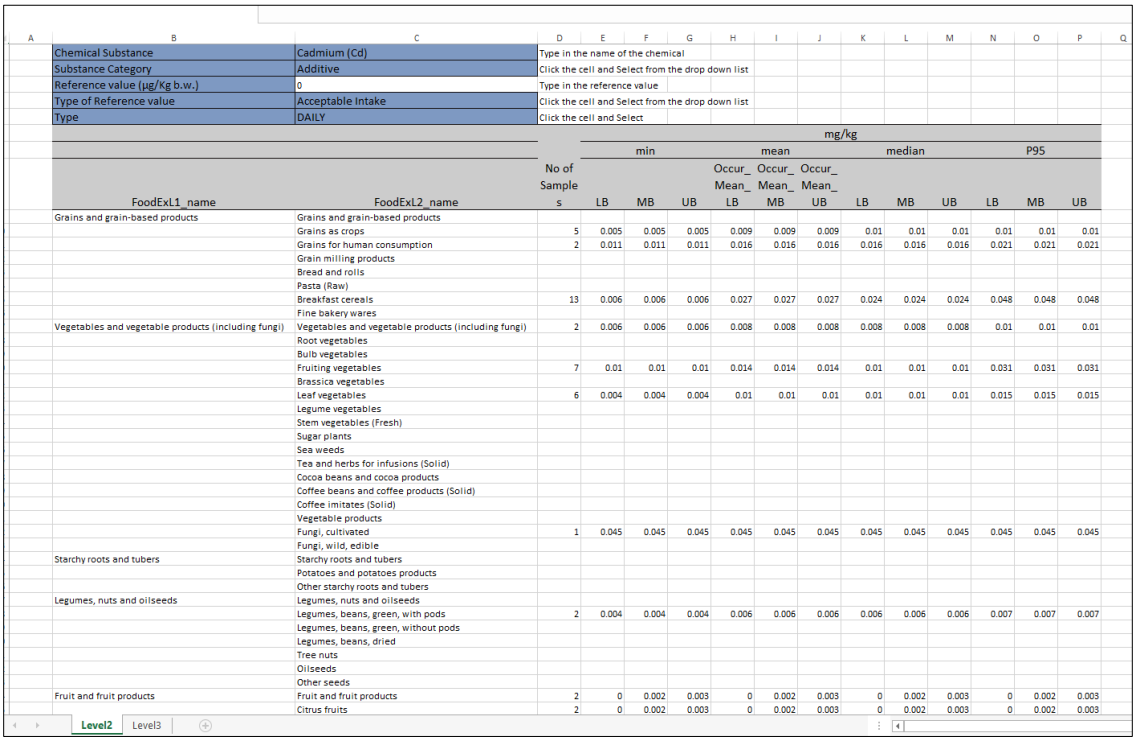


Figure 10 Download excel template



Chemical Substance	Cadmium (Cd)	Type in the name of the chemical														
Substance Category	Additive	Click the cell and Select from the drop down list														
Reference value (µg/Kg b.w.)	0	Type in the reference value														
Type of Reference value	Acceptable Intake	Click the cell and Select from the drop down list														
Type	DAILY	Click the cell and Select														
			mg/kg													
			min			mean			median			P95				
FoodExL1_name	FoodExL2_name	No of Samples	LB	MB	UB	Occur_ Mean_ LB	Occur_ Mean_ MB	Occur_ Mean_ UB	LB	MB	UB	LB	MB	UB		
Grains and grain-based products	Grains and grain-based products															
	Grains as crops	5	0.005	0.005	0.005	0.009	0.009	0.009	0.01	0.01	0.01	0.01	0.01	0.01		
	Grains for human consumption	2	0.011	0.011	0.011	0.016	0.016	0.016	0.016	0.016	0.016	0.021	0.021	0.021		
	Grain milling products															
	Bread and rolls															
	Pasta (Raw)															
	Breakfast cereals	13	0.006	0.006	0.006	0.027	0.027	0.027	0.024	0.024	0.024	0.048	0.048	0.048		
	Fine bakery wares															
Vegetables and vegetable products (including fungi)	Vegetables and vegetable products (including fungi)	2	0.006	0.006	0.006	0.008	0.008	0.008	0.008	0.008	0.008	0.01	0.01	0.01		
	Root vegetables															
	Bulb vegetables															
	Fruiting vegetables	7	0.01	0.01	0.01	0.014	0.014	0.014	0.01	0.01	0.01	0.031	0.031	0.031		
	Brassica vegetables															
	Leaf vegetables	6	0.004	0.004	0.004	0.01	0.01	0.01	0.01	0.01	0.01	0.015	0.015	0.015		
	Legume vegetables															
	Stem vegetables (Fresh)															
	Sugar plants															
	Sea weeds															
	Tea and herbs for infusions (Solid)															
	Cocoa beans and cocoa products															
	Coffee beans and coffee products (Solid)															
	Coffee imitates (Solid)															
	Vegetable products															
	Fungi, cultivated	1	0.045	0.045	0.045	0.045	0.045	0.045	0.045	0.045	0.045	0.045	0.045	0.045		
	Fungi, wild, edible															
Starchy roots and tubers	Starchy roots and tubers															
	Potatoes and potatoes products															
	Other starchy roots and tubers															
Legumes, nuts and oilseeds	Legumes, nuts and oilseeds															
	Legumes, beans, green, with pods	2	0.004	0.004	0.004	0.006	0.006	0.006	0.006	0.006	0.006	0.007	0.007	0.007		
	Legumes, beans, green, without pods															
	Legumes, beans, dried															
	Tree nuts															
	Oilseeds															
	Other seeds															
Fruit and fruit products	Fruit and fruit products	2	0	0.002	0.003	0	0.002	0.003	0	0.002	0.003	0	0.002	0.003		
	Citrus fruits	2	0	0.002	0.003	0	0.002	0.003	0	0.002	0.003	0	0.002	0.003		