

LIMS SHINY Application

v.0.1.0

A shiny application for creating ImproRisk occurrence templates

Description and User Manual

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Nicosia, Cyprus



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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

Aggregate LIMS data

Upload your occurrence raw data (or use the demo file)

Input Data

☒ Demo Data
☐ Upload Data

Edit the substance information accordingly

Substance: Cadmium (Cd)

Substance Category:

Reference Value (µg/ Kg bw):

Type of Reference Value:

Exposure type:

Filter your data

Choose columns to filter

Aggregated data **Raw data** FoodEx1 Data Description

FoodEx1 aggregation level:

Decimals?:

Dataset: 'demo_data_CD 2011-2013.xlsx'
Number of raw occurrence observations used: 721

[Download Excel Template](#)

	FOODEX_L1_DESC	FOODEX_L2_DESC	N	LB_min	MB_min	UB_min	LB_mean	MB_mean	UB_mean
	<input type="text" value="/All"/>	<input type="text" value="/All"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
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

Aggregate LIMS data

The screenshot shows a grey sidebar panel with three distinct sections separated by horizontal lines. The top section is titled 'Upload your occurrence raw data (or use the demo file)' and contains two radio buttons: 'Demo Data' (selected) and 'Upload Data'. The middle section is titled 'Edit the substance information accordingly' and contains several form fields: 'Substance: Cadmium (Cd)', 'Substance Category' (dropdown menu showing 'Additive'), 'Reference Value (µg/ Kg b.w.)' (text input with '0'), 'Type of Reference Value' (dropdown menu showing 'Acceptable Intake'), and 'Exposure type' (dropdown menu showing 'DAILY'). The bottom section is titled 'Filter your data' and contains a label 'Choose columns to filter' above a grey button that says 'Nothing selected'.

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

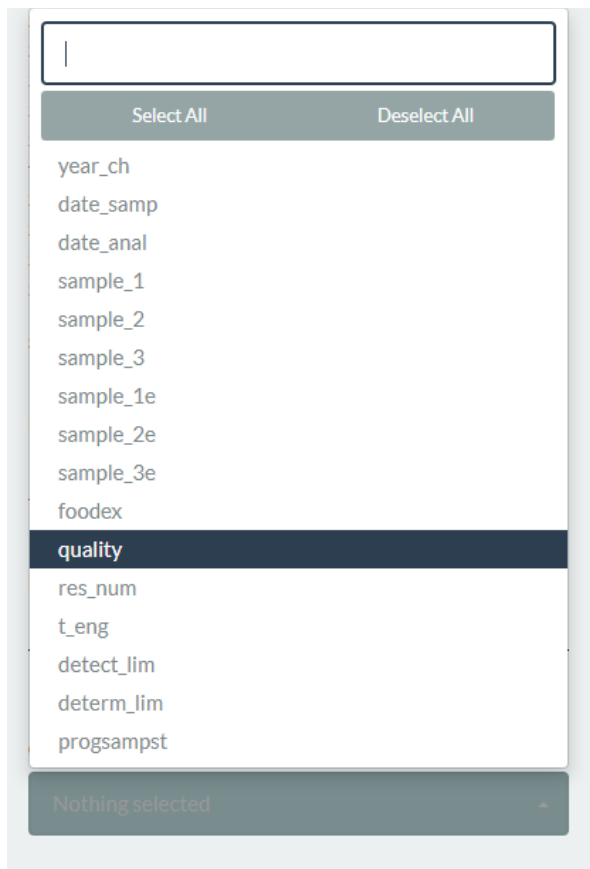
Section: Filter your data

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)

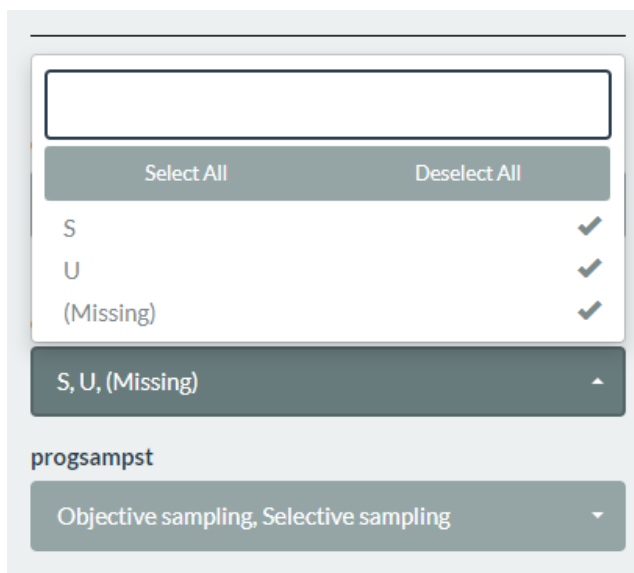
The appropriate filters appear for the user to select particular values from the selected columns. (Figure 4)

Figure 3 UI - select columns to filter on



A UI element for selecting columns to filter on. It features a search bar at the top, followed by two buttons: "Select All" and "Deselect All". Below these is a list of column names: year_ch, date_samp, date_anal, sample_1, sample_2, sample_3, sample_1e, sample_2e, sample_3e, foodex, **quality**, res_num, t_eng, detect_lim, determ_lim, and progsampst. The "quality" column is highlighted. At the bottom, there is a button labeled "Nothing selected" with a small upward arrow.

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



A UI element for selecting values from columns to filter the data. It features a search bar at the top, followed by two buttons: "Select All" and "Deselect All". Below these is a list of values: S, U, and (Missing), each with a checkmark to its right. Below this list is a button labeled "S, U, (Missing)" with a small upward arrow. At the bottom, there is a dropdown menu labeled "progsampst" with the text "Objective sampling, Selective sampling" and a downward arrow.

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

The screenshot shows the 'Aggregated data' tab with the following components:

- FoodEx1 aggregation level:** Buttons for 'Level 2' and 'Level 3'.
- Decimals?:** A text input field containing the value '3'.
- Dataset:** 'demo_data_CD 2011-2013.xlsx'
- Number of raw occurrence observations used:** 721
- Download Excel Template:** A button with a download icon.
- Table:** A table with 10 columns: FOODEX_L1_DESC, FOODEX_L2_DESC, N, LB_min, MB_min, UB_min, LB_mean, MB_mean, and UB_mean. It contains 7 rows of data for grain-based products.

	FOODEX_L1_DESC	FOODEX_L2_DESC	N	LB_min	MB_min	UB_min	LB_mean	MB_mean	UB_mean
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

Aggregated data

Raw data

FoodEx1

Data Description

Search:

year_ch	date_samp	date_anal	sample_1	sample_2	sample_3	sample_1e	sample_2e	sample_3e
			All	All	All	All		All
1	2011	2011-01-20	2011-01-28	ΨΑΡΙΑ,ΨΑΡΙΚΑ & ΠΡΟΙΟΝΤΑ	ΚΑΤΕΨΥΓΜΕΝΑ ΨΑΡΙΑ/ΨΑΡΙΚΑ	(Missing)	FISH & FISH PRODUCTS	FROZEN FISH (Missing)
2	2011	2011-01-20	2011-01-28	ΨΑΡΙΑ,ΨΑΡΙΚΑ & ΠΡΟΙΟΝΤΑ	ΚΑΤΕΨΥΓΜΕΝΑ ΨΑΡΙΑ/ΨΑΡΙΚΑ	(Missing)	FISH & FISH PRODUCTS	FROZEN FISH (Missing)
3	2011	2011-01-20	2011-01-28	ΨΑΡΙΑ,ΨΑΡΙΚΑ & ΠΡΟΙΟΝΤΑ	ΚΑΤΕΨΥΓΜΕΝΑ ΨΑΡΙΑ/ΨΑΡΙΚΑ	(Missing)	FISH & FISH PRODUCTS	FROZEN FISH (Missing)
4	2011	2011-01-20	2011-01-28	ΨΑΡΙΑ,ΨΑΡΙΚΑ & ΠΡΟΙΟΝΤΑ	ΚΑΤΕΨΥΓΜΕΝΑ ΨΑΡΙΑ/ΨΑΡΙΚΑ	(Missing)	FISH & FISH PRODUCTS	FROZEN FISH (Missing)
5	2011	2011-01-20	2011-01-28	ΨΑΡΙΑ,ΨΑΡΙΚΑ & ΠΡΟΙΟΝΤΑ	ΚΑΤΕΨΥΓΜΕΝΑ ΨΑΡΙΑ/ΨΑΡΙΚΑ	(Missing)	FISH & FISH PRODUCTS	FROZEN FISH (Missing)
6	2011	2011-01-26	2011-02-01	ΨΑΡΙΑ,ΨΑΡΙΚΑ & ΠΡΟΙΟΝΤΑ	ΚΑΤΕΨΥΓΜΕΝΑ ΨΑΡΙΑ/ΨΑΡΙΚΑ	(Missing)	FISH & FISH PRODUCTS	FROZEN FISH (Missing)

<

>

Showing 1 to 721 of 721 entries

FoodEx1

This Tab shows the FoodEx1 categorisation hierarchy. The table displays the FoodEx1 code and description on Level 4 through 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	FOODEX_L1_DESC
	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 and grain-based products
2	A.01.000002	Grains as crops	A.01.000002	Grains as crops	A.01.000002	Grains as crops	A.01.000001	Grains and grain-based products
3	A.01.000003	Wheat grain crop	A.01.000003	Wheat grain crop	A.01.000002	Grains as crops	A.01.000001	Grains and grain-based products
4	A.01.000004	Barley grain	A.01.000004	Barley grain	A.01.000002	Grains as crops	A.01.000001	Grains and grain-based products
5	A.01.000005	Corn grain	A.01.000005	Corn grain	A.01.000002	Grains as crops	A.01.000001	Grains and grain-based products
6	A.01.000006	Rye grain	A.01.000006	Rye grain	A.01.000002	Grains as crops	A.01.000001	Grains and grain-based products
7	A.01.000007	Spelt grain	A.01.000007	Spelt grain	A.01.000002	Grains as crops	A.01.000001	Grains and grain-based products
8	A.01.000008	Buckwheat grain	A.01.000008	Buckwheat grain	A.01.000002	Grains as crops	A.01.000001	Grains and grain-based products
9	A.01.000009	Millet grain	A.01.000009	Millet grain	A.01.000002	Grains as crops	A.01.000001	Grains and grain-based products
10	A.01.000010	Oats, grain	A.01.000010	Oats, grain	A.01.000002	Grains as crops	A.01.000001	Grains and grain-based products

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

Aggregated dataRaw dataFoodEx1Data Description

A description of the columns in the dataset

The table shows what each column in the data represents

Search:

	var_id	var_label	Required
	<input type="text" value="All"/>	<input type="text" value="All"/>	<input type="text" value="['Yes']"/>
3	year_ch	Year of Analysis	Yes
6	date_samp		Yes
7	date_anal	Date of Analysis	Yes
9	sample_1		Yes
10	sample_2		Yes
11	sample_3		Yes
12	sample_1e		Yes
13	sample_2e		Yes
14	sample_3e		Yes
16	foodex		Yes
17	t_eng	Substance	Yes
25	quality	Quality	Yes
47	progsampst	Sampling strategy	Yes
63	res_num	Occurrence	Yes
68	detect_lim	Limit of Detection (LOD)	Yes
69	determ_lim	Limit of Determination (LOQ)	Yes

Showing 1 to 16 of 16 entries (filtered from 72 total entries)

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

The screenshot shows the 'Aggregated data' tab with the following details:

- Aggregated data | Raw data | FoodEx1 | Data Description
- FoodEx1 aggregation level: Level 2 (selected), Level 3
- Decimals?: 3
- Dataset: 'demo_data_CD 2011-2013.xlsx'
- Number of raw occurrence observations used: 721
- Download Excel Template** (button circled in red)

Figure 10 Download excel template

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
	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				
			No of Sample s	Occur_	Occur_	Occur_									
				Mean_	Mean_	Mean_									
	FoodExL1_name	FoodExL2_name		LB	MB	UB	LB	MB	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
	Level2	Level3													