



FACET Exposure Assessment Tool

User Manual

Version 3.0.2

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1. Contents

1.	Contents	2
2.	System Requirements	4
3.	Release Notes	4
4.	Overview.....	5
	Data Structures	5
	Terms.....	6
	Home Tab	7
	Assessments Tab	8
5.	Assessment Navigation and Organisation	11
	Creating a new folder	11
	Renaming a folder	12
	Deleting a Folder	12
6.	Running an Assessment.....	13
	Select Assessment Type	14
	Select Substance	14
	Searching for a Substance	15
	Flavourings	16
	Additives.....	16
	Packaging Migrant.....	17
	Search Results	18
	Using Custom Concentration Data.....	19
	Select Concentration Data	19
	Select Pack Types	20
	Food Categories	21
	Select Survey	24
	Select Population Filters.....	26
	Assessment Options.....	26
	Flavouring Assessment Options	27
	Additive Assessment Options.....	29
	Packaging Assessment Options.....	29
	Advanced Options	30
	Assessment Summary	32
	Renaming an Assessment	32
	Deleting an Assessment	32
	Viewing the Results Report.....	33
	Viewing Graphs of the Assessment Results	33
	Viewing Graphs	34
	Viewing Data Only	38
	Viewing All Results	39
7.	FACET Data	41
	Flags.....	42
	Food Categories	42
	Migration Information	45
	Substances	47
	Flavourings	47
	Flavourings Info.....	48

Screening Calculations	50
Additives.....	50
Additive Info.....	51
Additive Ingredient Distributions.....	53
Packaging	54
Surveys	56
8. My Data Tab	58
Managing Data	58
Navigating about the data manager	58
Creating a new folder	59
Renaming a folder.....	59
Deleting a folder	59
Create New Table	59
Entering data.....	61
Concentrations.....	61
Presence Probabilities	61
Food Codes	62
Flag Settings.....	63
9. New Packaging Wizard	64
New Pack Type	64
Limitations of the migration model	70
Metal Pack Type	71
10. New Substance Wizard.....	76
New substance (Non Metal) and NIAS (Non-Metal)	77
Replace Existing Substance/NIAS Associated with an Existing Substance	78
Select Materials Containing Substance/NIAS	80
New Substance (Metal) and NIAS (Metal)	82
The output of the New Substance Wizard	82
11. Troubleshooting	83
Restart the software	83
Close FACET using the Task Manager.....	83
Uninstall and reinstall FACET	83

2. System Requirements

This software will run on machines using the Microsoft Windows XP®, Windows Vista®, or Windows 7® operating systems. The user must have administrator privileges on their PC to install this software. If using Windows 10, the user must have administrator rights to use FACET 3.0.2. This is because the software needs read/write access to specific computer files and a security update in Windows 10 has made these specific files read/write only to those who have administrator status.

Approximately 1GB of disk space is required for installation of the software. A processor with at least 1GHz clock speed and 1GB of RAM is recommended.

For optimum use of the software, it is recommended to use a display with resolution of 1024 x 768 or higher.

3. Release Notes

This software is the final implementation of the workflow, features, and functionality for the FACET exposure assessment tool. This workflow has been refined and modified over time based on consortium feedback from FACET versions 1.0 (January 2010), 1.2 (May 2010), 1.4 (October 2010), 1.5 (April 2011), 1.6 (February 2012), 1.7 (August 2012), 1.8 (October 2012), 1.9 (November 2012), 2.0 (August 2013), 2.0.6 (November 2013), 3.0.2 (October 2016) . The software contains all databases and models gathered and developed over the course of the FACET project.

4. Overview

The software is implemented in a four panel layout. These four panels, referred to as “tabs”, are:

- **Home:** dashboard providing program status and basic program information.
- **Assessments:** interface to view results from completed assessments or the status of assessments currently running.
- **FACET Data:** interface to view non-sensitive data that has been pre-installed in the software.
- **My Data:** interface to view data that the user has loaded into the FACET program.

On starting the software, the “Home” tab will be presented.

Navigate between tabs by clicking on the tab name (“Home”, “Assessments”, “FACET Data”, “My Data”) near the top left of the program window.

By default the program window opens to a default size. You can resize the window to the desired size. To ensure adequate display of all features, there is a minimum allowed size for the window.

Data Structures

The FACET software supports a number of probabilistic data structures in the form of parametric and empirical distributions. In general, these can be used in place of point values for inputs such as chemical concentrations, contact areas, etc. A table of the possible options is below.

Distribution Type	Number Of Arguments	Arguments	Example1
Uniform Distribution Discrete	Any	Comma separated values	choice(0, 1, 1, 2, 3, 5, 8, 13)
Weighted Distribution Discrete	Any	Comma separated values	weighted(0.2, 3.14, 0.2, 1.618, 0.6, 2.718)
Uniform Continuous Distribution	2	Min, Max	uniform(1, 5)
Triangular Distribution	3	Min, Typical, Max	triangular(0, 1, 2)
Normal Distribution	2	Mean, S. D.	gaussian(23, 1)
Normal Distribution With Bounds	4	Mean, S. D., min, max	gaussian(23, 1, 22, 24)
Lognormal Distribution	2	Mean and S. D. of underlying normal	lognormal(74, 10)
Weibull Distribution	2	Shape, Scale	weibull(1, 1.5)
Chi Squared Distribution	1	Degrees of Freedom	chisquared(2)
Gamma Distribution	2	Shape, Scale	gamma(9, 0.5)

The “choice” distribution is used when a set of values are all equally likely.

The “weighted” distribution is used when different values occur with a given weight or frequency, in the form of (weight, value, weight, value,...). Note that the sum of the weights does not need to be less than zero or sum to one.

In general, these can be nested within each other, e.g. the individual elements of a weighted distribution can be composed of normal distributions: `weighted(0.2, gaussian(2, 5), 0.8, gaussian(1,3))`.

Terms

Set-off is the transfer of substances present in inks or lacquers (Material Codes M21, M27 and all of their *children* codes), when used as outermost layers, to the innermost layer of a multilayer packaging material. This is to simulate what may happen during storage of the material prior to being placed in contact with food. The Set off in FACET is set to 20%. Specifically, 20% of the mass of the substance in a material code beginning with M21, or M27, will, prior to simulating migration, be added to the initial concentration of that migrant in the innermost layer and effectively be distributed in the thickness of that innermost layer, thus making it available for migration to the food.

Home Tab

The Home tab comprises:

- **Project Summary:** In the centre of the page is a brief summary of the FACET project.
- **Quick start buttons:** Below the project summary there are three quick start buttons. These are:
 - *Create New Assessment:* This launches the FACET Assessment Wizard that guides users through the steps required to perform an assessment. Clicking on this button is equivalent to clicking on the “New Assessment” button in the toolbar at the top of the screen.
 - *Go to FACET Data:* Clicking on this button will bring users to the “FACET Data” tab, where users can browse through non-confidential data built into the program. Clicking on this button is equivalent to clicking on the “FACET Data” tab.
 - *Go to My Data:* Clicking on this button opens the “My Data” tab, where users can browse and edit their own custom data for use in an assessment. Clicking on this button is equivalent to clicking on the “My Data” tab.

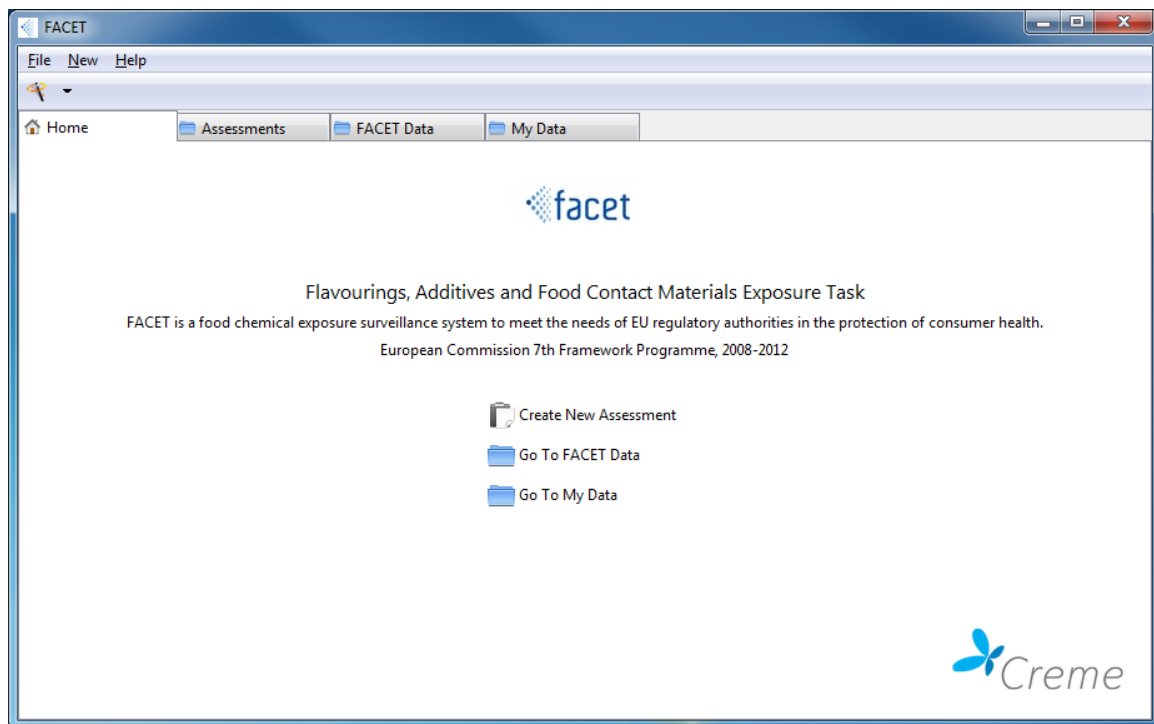


Figure 1: The Home Tab

Assessments Tab

The assessment tab is where all assessments are stored, and is similar to any file management system. The view is implemented in a three panel layout.

The left-hand pane shows a tree structure that shows how the user's folders are organised.

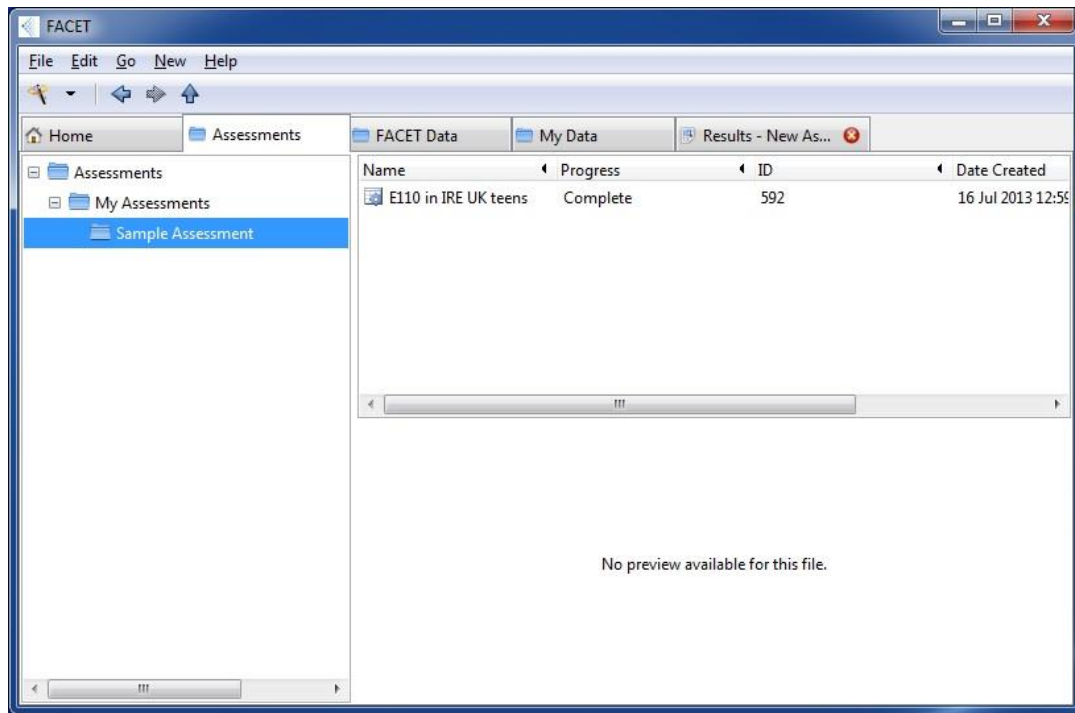


Figure 2: The assessment tab

The top right panel shows the contents of the folders, which are assessments. The assessments are presented in a list view, and the following fields are displayed:

- **Name:** The name given to the assessment by the user.
- **Progress:** This is a progress bar showing what percentage of the assessment has been completed.
- **ID:** The unique ID number of the assessment.
- **Date Created:** The date the assessment was run.
- **Date Accessed:** The date the assessment was last viewed.

Name	Progress	ID	Date Created
E110 in IRE UK teens	Complete	592	16 Jul 2013 12:59

Figure 3: List view of assessment

The bottom right panel provides the status and details of whatever assessment is selected in the top right pane. It also provides buttons that allow the user to view the results of the selected assessment ("View All Results") view the graphs of the assessment ("View Graphs") or view the report generated by the assessment ("View Report"). Descriptive fields appear in the assessment summary (Figure 4).

The screenshot shows the FACET software window. On the left is a navigation pane with 'Home', 'Assessments', and 'My Assessments'. The main area displays a table of assessments. The second row is selected, showing details for 'Sample Ax: 9024 in French males < 20 yr old (All foods)'. Below the table are buttons for 'View All Results', 'View Graphs', and 'View Report'. At the bottom is an 'Assessment Summary' section with the following details:

ID:	625						
Name:	Sample Ax: 9024 in French males < 20 yr old (All foods)						
Description:	Fitted distribution - lognormal						
Type:	Flavouring (FEMA)						
Substance:	9024 - Isopentyl acetate						
Survey(s):	<table border="1"> <tr> <th>Name</th> <th>Filtered Population Size</th> <th>Simulated Population Size</th> </tr> <tr> <td>France INCA 2</td> <td>740</td> <td>740</td> </tr> </table>	Name	Filtered Population Size	Simulated Population Size	France INCA 2	740	740
Name	Filtered Population Size	Simulated Population Size					
France INCA 2	740	740					
Population Filters:	Gender: Male Age: between 0 and 20						
Date Submitted:	8 Aug 2012 12:35						
Software Version:	1.7b2						

Figure 4: Summary of assessment

- **ID:** This is a unique identifier of the assessment within the program.
- **Name:** The name given to the assessment by the user.
- **Description:** Any further description the user included in the assessment.
- **Type:** The type of the assessment (Additive, Flavouring, or Packaging Migrant).

- **Substance:** The substance used in the assessment.
- **Survey(s):** The survey(s) used in the assessment, the number of subjects in the original survey (*Filtered Population Size*), and the number of subjects simulated (*Simulated Population Size*).
- **Population Filters:** Any population filters that may have been used in the assessment.
- **Date Submitted:** The date on which the assessment was performed.
- **Software Version:** The version of the software used to perform the assessment.

5. Assessment Navigation and Organisation

To navigate about the assessment manager, there are a few options;

1. Use the “Back”, “Forward”, and “Up” buttons in the tool bar.
2. Click on the desired folder to view in the folder tree in the left panel. The subfolders contained in a folder can be viewed by clicking on the plus symbol next to a folder in the left hand pane.
3. Double-clicking on the folder or assessment in the top right pane.

The folder structure in the left hand panel will expand or collapse to show what stage of the assessment manager the user is at.

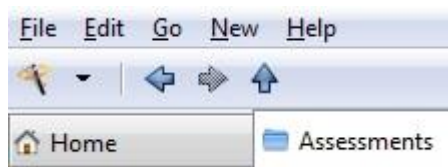


Figure 5: Back/forward/up arrows

Creating a new folder

1. To create a new folder, select “Create Folder” from the file menu.
2. This will bring up a dialogue box to name the new folder and click ok to save.

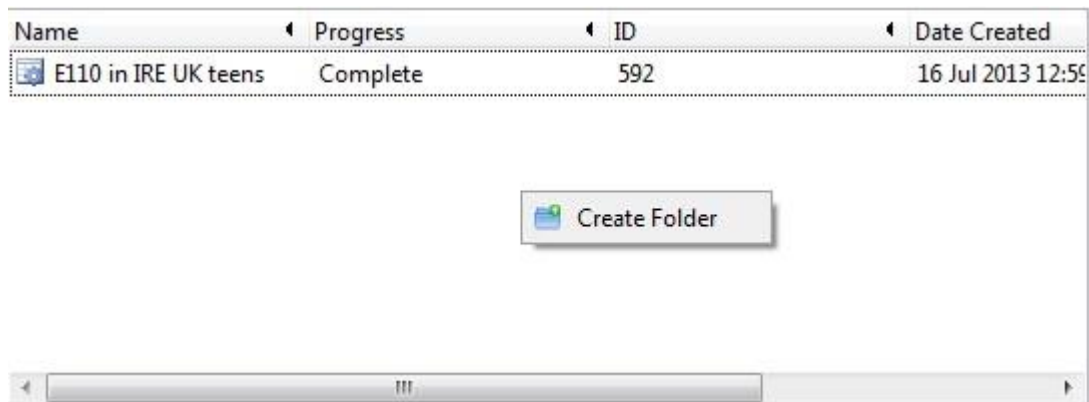


Figure 6: Creating a new folder

Renaming a folder

1. To rename a folder, right click on the folder and select “Rename”. Alternatively, select the folder and choose “Rename” from the Edit menu (Figure 7).
2. This will bring up a dialogue box into which the new name of the folder can be entered. Enter the new name of the folder into the dialogue box and click on “Rename”.

Deleting a Folder

1. To delete a folder, right click on the folder to delete and select “Delete” from the context menu (Figure 7).
2. Alternatively, select the folder to delete and choose “Delete” from the Edit menu.

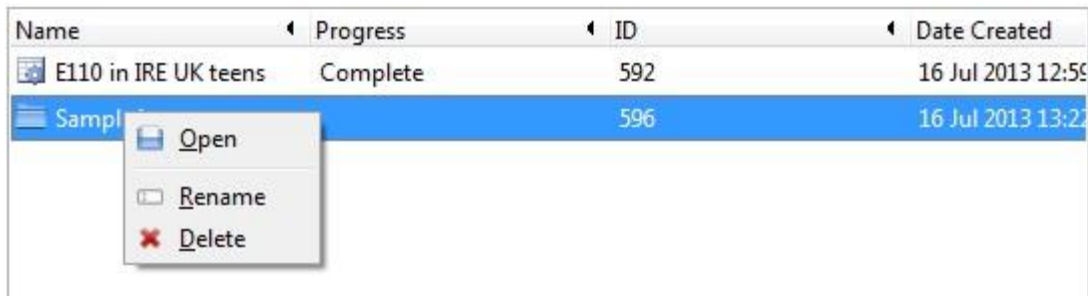


Figure 7: Renaming/deleting a folder

6. Running an Assessment

The New Assessment Wizard provides the workflow to set up a new exposure assessment. This can be selected from the file menu by selecting the “New” menu and then clicking on “New Assessment” (Figure 8). Alternatively, click on the wizard icon in the tool bar and select “New Assessment” (Figure 9), or select “Create New Assessment” in the home tab. When selected, the Assessment Wizard appears in a new window.

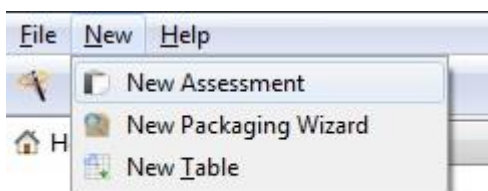


Figure 8: New assessment

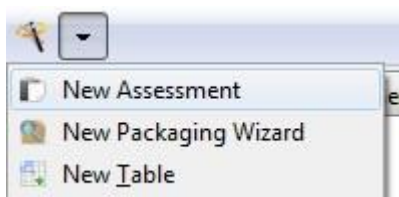


Figure 9: New assessment (2)

Depending on the assessment type, there are eight or nine steps to complete:

1. **Select Assessment Type:** Choose the type of assessment; flavouring, additive, or packaging migrant.
2. **Select Flavouring/Additive/Substance:** Choose substance to which exposure is to be estimated. This step also allows users to choose between using pre-installed FACET data or user-specified concentration data.
3. **Select Concentration Data:** For a flavourings assessment this also allows the user to choose which of the pre-installed sources of concentration to use.
4. **Select Pack Types:** For packaging assessments only. Choose all or specific packaging types to use in an assessment.
5. **Select Food Categories:** Choose all or specific food categories.
6. **Select Surveys:** Choose between different consumption surveys and specific ages or genders.
7. **Assessment Options:** Choose assessment name, description, output statistics and other options for the assessment.
8. **Assessment Summary:** Summary of selections for this assessment, and proceed to submit assessment.

Users are guided through these steps in sequential order. Proceed to the next step by clicking the “Next” button at the bottom left of the program window. Clicking the “Next” button without

successfully completing the current step will display a red “X” next to that step to indicate that it has not been successfully completed.

One can also navigate between the already completed steps by either:

- Clicking “Next” at the bottom right of the program window.
- Clicking “Previous” that appears in the bottom right of the Assessment Wizard window.
- Clicking the stage name buttons at the left hand of the program window.

It is not possible to proceed to a later step using these stage name buttons without having already completed all steps previous to this later step.

Select Assessment Type

In Step 1, choose an exposure assessment type; a flavouring, additive, or packaging migrant, by clicking on the appropriate image above the desired assessment type (Figure 10).

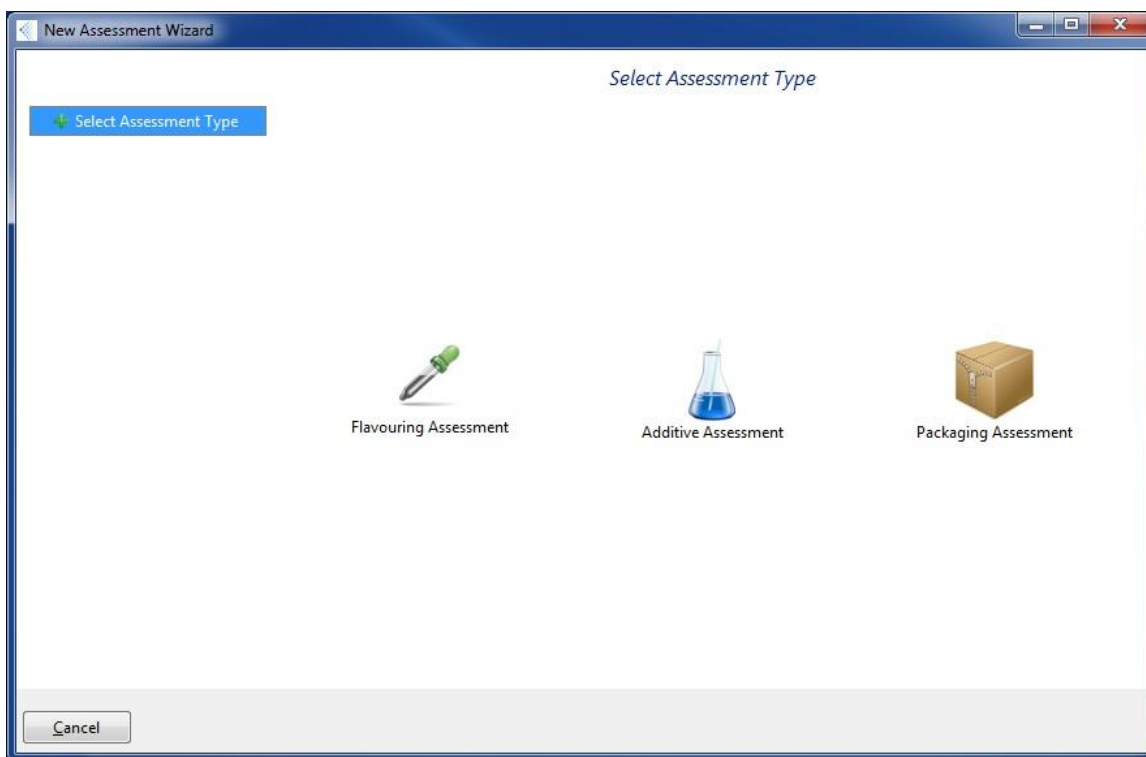


Figure 10: Selecting an assessment type

Select Substance

The target substance for the assessment can be chosen from the list of built-in substances displayed at this step. By default, the option “Use pre-installed FACET data” is selected:

☒ Use pre-installed FACET data.

This is simply done by clicking anywhere on the row containing the substance of interest, or on the radio button next to the substance ID.

The list of substances may also be searched to find the substance of interest. This search procedure is explained in detail below for each assessment type.

Alternatively, one can use their own table of concentration data to use in an assessment, by selecting the “Use my concentration data” option:

☒ Use my concentration data

This involves populating a table of concentrations beforehand. See “New Table Wizard” in the “My Data” section of the manual for more details on how to do this.

Searching for a Substance

New Assessment Wizard

Select Flavouring

☒ Select Assessment Type
☒ **Select Flavouring**
 Select Concentration Data
 Select Food Categories
 Select Surveys
 Assessment Options
 Assessment Summary

☒ Use pre-installed FACET data.
 Search: Flavis Number Clear

FI No	Flavis Name	CAS Number	CoE	Flavis Number	Name(s)	Targ	In Re
2015	Menthol	89-78-1	63			No	Yes
2016	Borneol	507-70-0	64			No	Yes
2017	Cinnamyl alcohol	104-54-1	65			No	Yes
2018	Nerolidol	7212-44-4	67			No	Yes
2019	2-Phenylethan-1-ol	60-12-8	68			No	Yes
2020	Hex-2-en-1-ol	2305-21-7	69	2562	1354	No	Yes
2021	Heptan-1-ol	111-70-6	70	2548	94	No	Yes
2022	Octan-2-ol	123-96-6	71	2801	289	No	Yes

No substances selected.

☐ Use my concentration data
 Select Concentration Table:

- My Data
 - My Additive Data
 - My Flavouring Data
 - My Migration Data
 - My Packaging Data
 - My Pre-Population Data

Name Date Created Date Accessed

Figure 11: Available search fields for Flavourings

Flavourings

The available search fields for substances assessed as flavourings are Flavis Number, CAS Number, Name(s), CoE Number, FEMA number, and JECFA number. “Instant searching” is enabled in all fields. That is, as search criteria is entered into the search box, search results are returned at each key stroke. A new search can be performed by either deleting what is in the search box or clicking on the “Clear Search” button.

- **Flavis Number:** Numeric field, the number assigned by FLAVIS – the EU Flavour Information System. This is strictly a four or five digit number and is the only unique identifier of flavourings in the FACET project.
- **CAS Number:** This is strictly of the form [up to 7 digits]-[2 digits]-[1 digit], e.g. “64-17-5”, or “0000064-17-5”.
- **Name(s):** This searches both the Flavis Name and Alternative Name fields.
- **CoE Number:** *Council of Europe Number*. This is strictly a numeric field, but can be any length.
- **FEMA Number:** Flavour and Extract Manufacturers Association. This is strictly a numeric field, but can be any length.
- **JECFA Number:** Joint FAO/WHO Expert Committee on Food Additives. This is strictly a numeric field, but can be any length.

Additives

The available search fields for substances assessed as additives are E Number and Name(s). “Instant searching” is enabled in both fields. That is, as one enters search criteria into the search box, search results are returned at each key stroke. A new search can be performed by either deleting what is in the search box or clicking on the “Clear Search” button. The displayed table also indicates whether or not an MPL value is available for that additive.

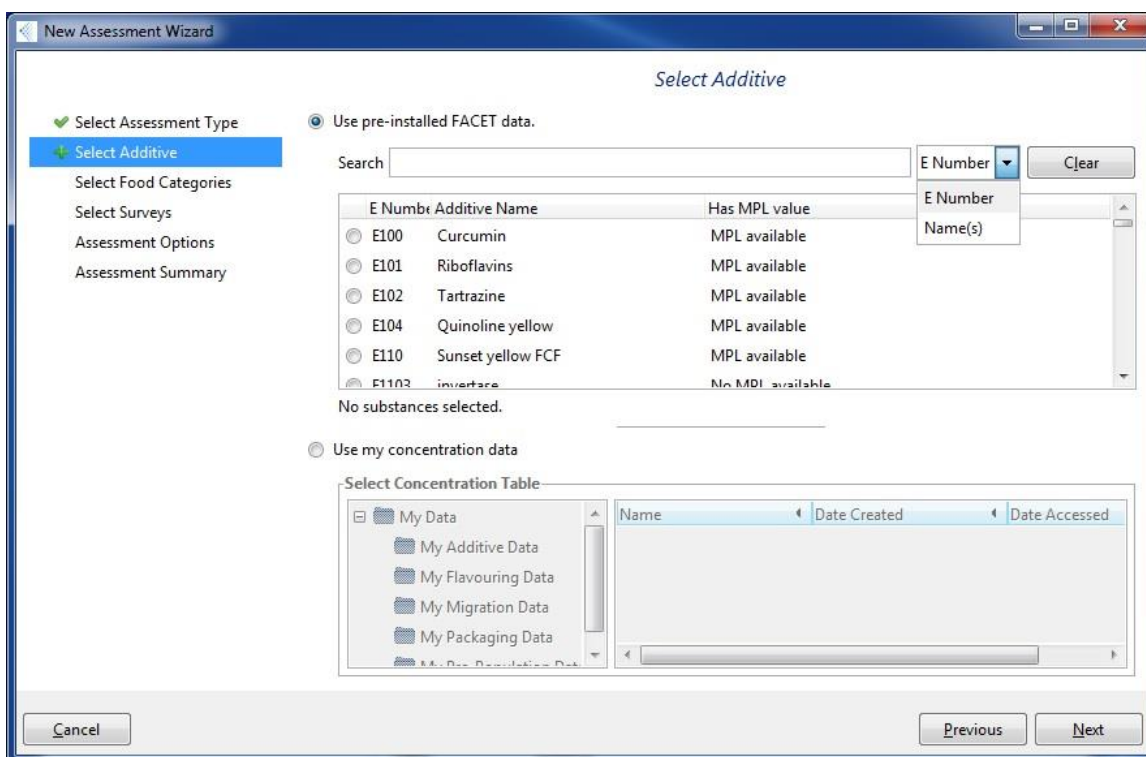


Figure 12: Available search fields for Additives

- **E Number:** This field takes a combination of numbers and letters.
- **Name(s):** This searches the additive name field.

Packaging Migrant

Note that only substances that have been pre-populated using the migration model (Pre-Population Wizard) will appear here. The available search fields for substances assessed as packaging migrants are FACET ID, CAS Number, Name(s), Molecular Formula, and Molecular Weight. The CAS Number field has the same options as those available when searching for flavourings, as described above. “Instant searching” is enabled in all fields. That is, as search criteria is entered into the search box, search results are returned at each key stroke. A new search can be performed by either deleting what is in the search box or clicking on the “Clear Search” button.

- **FACET ID:** This is strictly a four digit number with no leading zeros, e.g. “1021”.
- **CAS Number:** This is strictly of the form [up to 7 digits]-[2 digits]-[1 digit], e.g. “64-17-5”, or “0000064-17-5”.
- **Name(s):** This searches both the Chemical Name and Alternative Name fields.

- **Molecular Formula:** This field takes a combination of letters and numbers.
- **Molecular Weight:** This is strictly a number, with up to a maximum of 3 decimal places, e.g. “60”, “301.5”, “72.345”.
- **Pre-populated:** For each pre-populated substance this field is set to WITHOUT, WITH or BOTH. The first option, WITHOUT, means that the substance was pre-populated without set-off. In the second case, WITH means that the substance was pre-populated with set-off. The third option, BOTH, signifies that the substance was pre-populated both with and without set-off.

New Assessment Wizard

Select Migrant

☒ Select Assessment Type

☒ Use pre-installed FACET data.

Search FACET ID

FACET ID	CAS Number	Chemical Name	Alternative N
<input checked="" type="radio"/> 1401	0000103-23-1	Adipic acid, bis(2-ethylhexyl) ester	Adipic acid c
<input checked="" type="radio"/> 1443	0000119-61-9	Benzophenone	Benzene, ber

No substances selected.

☐ Use my concentration data

Select Concentration Table

☒ My Data

- ☐ My Additive Data
- ☐ My Flavouring Data
- ☐ My Migration Data
- ☐ My Packaging Data

Name	Date Created	Date Accessed
------	--------------	---------------

☐ Use in combination with pre-installed FACET data

Figure 13: Searching for packaging substances.

Search Results

The search results are returned instantaneously after each keystroke. Select a substance from the list and click on the “Next” button.

Using Custom Concentration Data

This allows users to use a table of pre-loaded concentration data. The folders in the My Data tab will be made visible and available for selection. Select one and click “Next”.

The substance used will be unique to the table created. Any food categories created in the table will appear as options in the next step of the wizard, so not all food categories in the table need be used in an assessment.

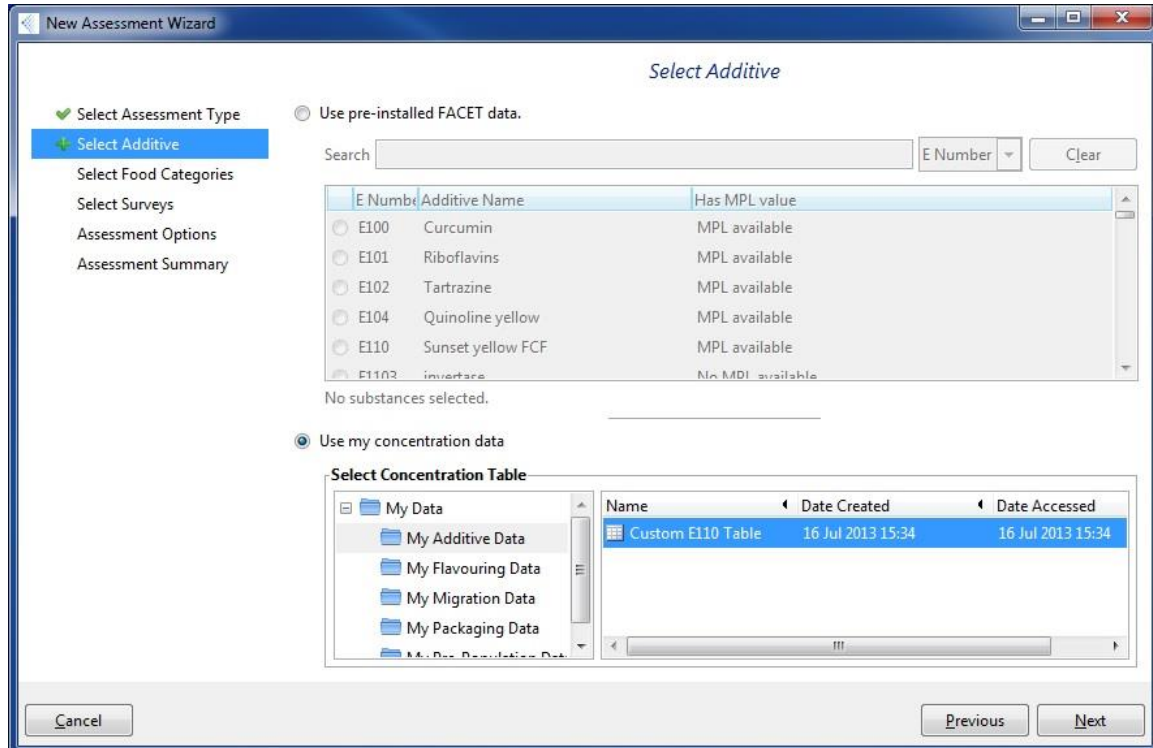


Figure 14: Using custom concentration data

Select Concentration Data

If the substance of interest is a flavouring, the FACET data is divided into eight options:

- Council of Europe, 2000
- EFFA (use levels provided to EFSA)
- FEMA (reported in Fenaroli's Handbook 2005)
- Young et al., 2006
- IOFI JECFA 2006 (use levels provided to JECFA)
- IOFI JECFA 2007 (use levels provided to JECFA)
- IOFI DG SANCO 2007 (use levels provided to JECFA)
- IOFI JECFA 2010 (use levels provided to FACET)

Each dataset has a set of warnings associated with it that the user should consider before performing an exposure assessment with that particular dataset.

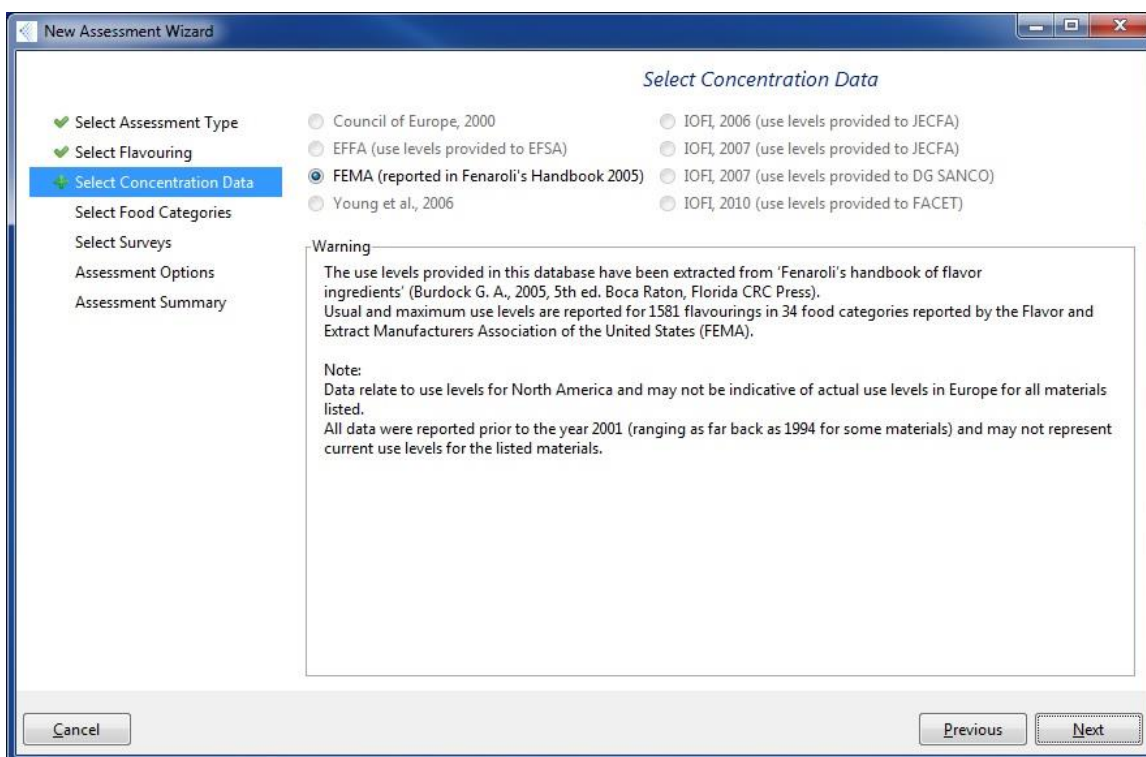


Figure 15: Selecting the source of concentration data

Select Pack Types

If the substance of interest is a packaging migrant, one can select all packaging types or specify which particular types to perform the assessment with. If the substance is a flavouring or additive, this step is skipped.

By default, no pack types are selected for this step. One can select/deselect all packs by clicking on the checkbox at the top left hand corner of this step. The pack types are arranged into four groups; "Main", "Closure", "Outer" and "Insert". To view the contents of a particular pack type, simply click on the plus symbol to the left of that pack type. When pack category is selected, all entries in the tier below are automatically selected too. Tri-state checkboxes are also enabled, whereby a square is shown in the checkbox to indicate the box is neither checked nor unchecked. This is the case when some, but not all, elements of a particular category are checked.

Instant searching is enabled for the pack types. That is, as one enters search criteria into the search box, search results are returned at each key stroke. Sections that match the search are returned highlighted in yellow. To search and select multiple pack types, simply search, select packs of interest, and search again. The pack types you selected will remain selected even if they are not displayed.

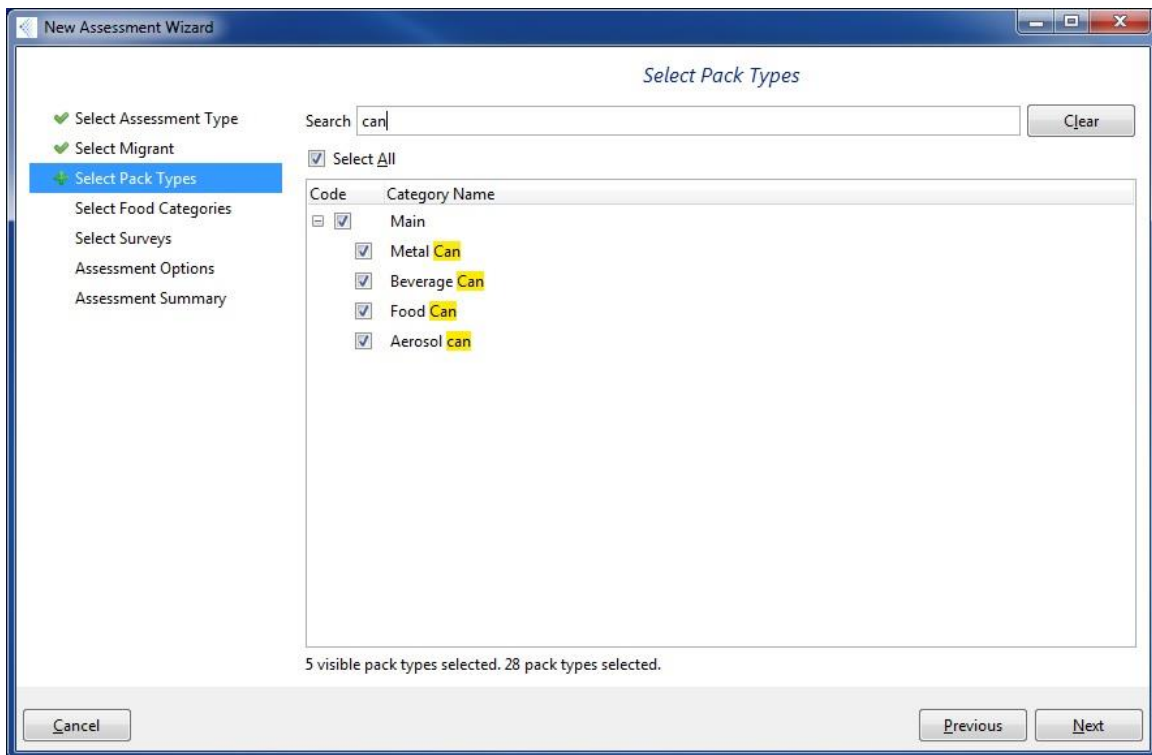


Figure 16: Searching for and selecting pack types.

Food Categories

Here one can select all food categories or specify which food categories to perform the assessment with.

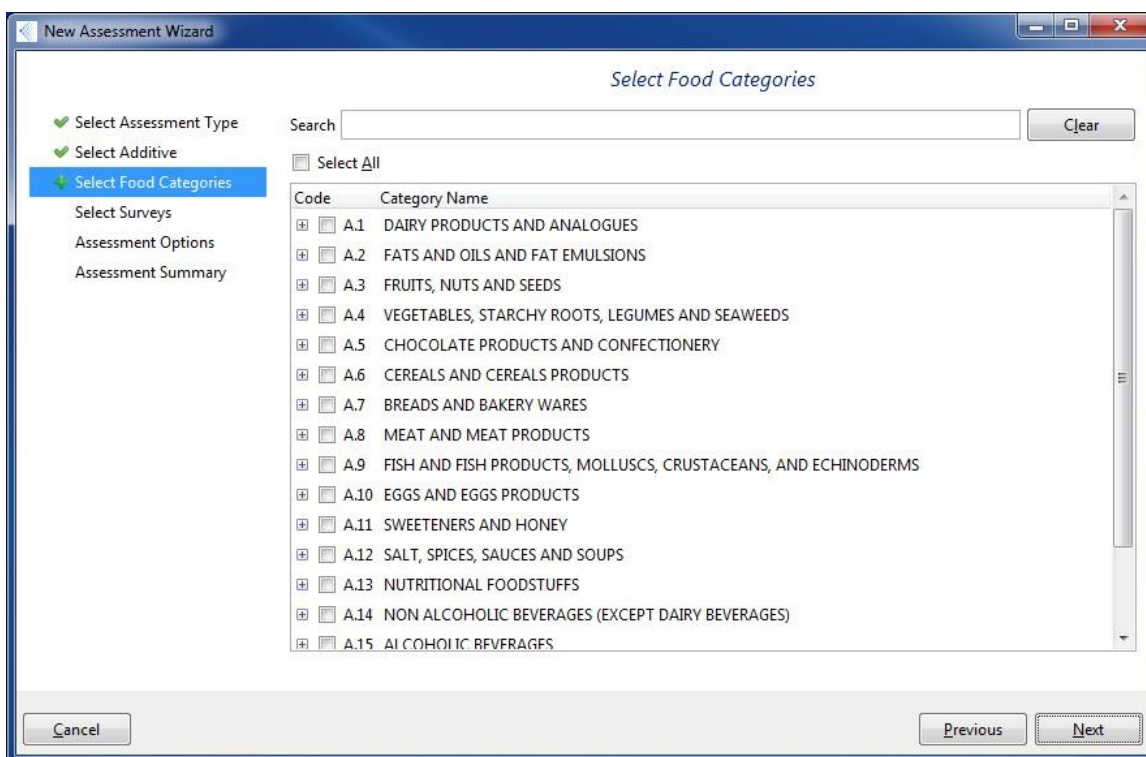


Figure 17: Select Food Categories

By default, no food categories are selected at this step. For all substances, the food groups are displayed (Figure 17) in 18 top level categories. The letter at the beginning of each food category indicates the type of substance being assessed (“A” for Additive, “F” for Flavouring, “P” for Packaging Migrant).

To select/deselect all categories, click on the “Select All” checkbox at the top right hand corner of the view. To move to a lower tier of a particular food category, simply click on the plus to the left of that category. If there are further tiers within that category, users can click on these to expand them further (Figure 18 and Figure 19).

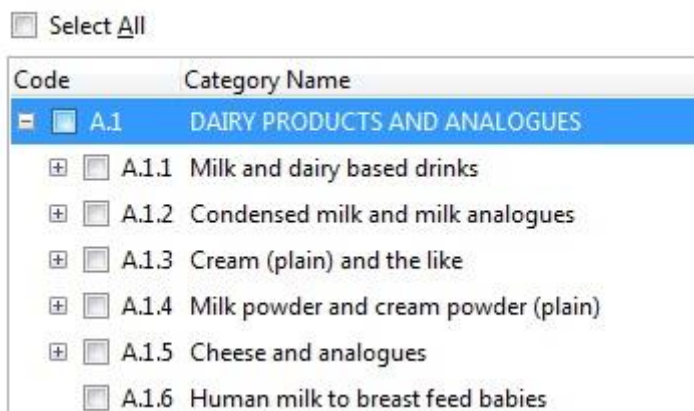


Figure 18: Select all box and expanded tier.

Code	Category Name
<input checked="" type="checkbox"/> A.1	DAIRY PRODUCTS AND ANALOGUES
<input checked="" type="checkbox"/> A.1.1	Milk and dairy based drinks
<input checked="" type="checkbox"/> A.1.1.1	Milk (plain)
<input type="checkbox"/> A.1.1.2	Buttermilk (plain)
<input type="checkbox"/> A.1.1.3	Dairy-based drinks
<input type="checkbox"/> A.1.2	Condensed milk and milk analogues
<input type="checkbox"/> A.1.3	Cream (plain) and the like
<input type="checkbox"/> A.1.4	Milk powder and cream powder (plain)

Figure 19: Further expanded tier and example of tri-state check box.

When a tier is selected, all entries in that tier below are automatically selected too. Tri-state checkboxes are also enabled, whereby a square is shown in the checkbox to indicate the box is neither checked nor unchecked. This is the case when some, but not all, elements of a particular category are checked.

Instant searching is enabled for the food groups. That is, as users enter search criteria into the search box, search results are returned at each key stroke. Sections that match the search are returned highlighted in yellow. To search and select multiple foods, simply search, select foods of interest, and search again. The selected foods will remain selected even if they are not displayed.

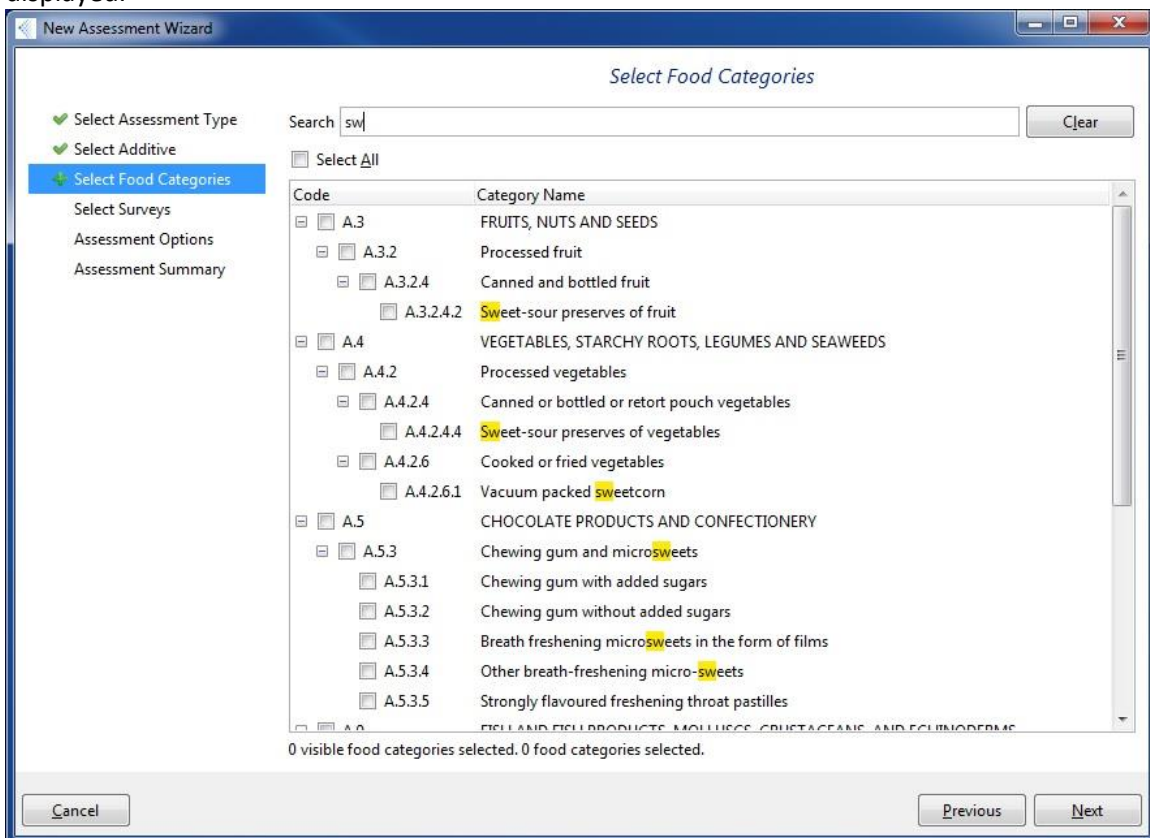


Figure 20: Search results are updated with every character entered

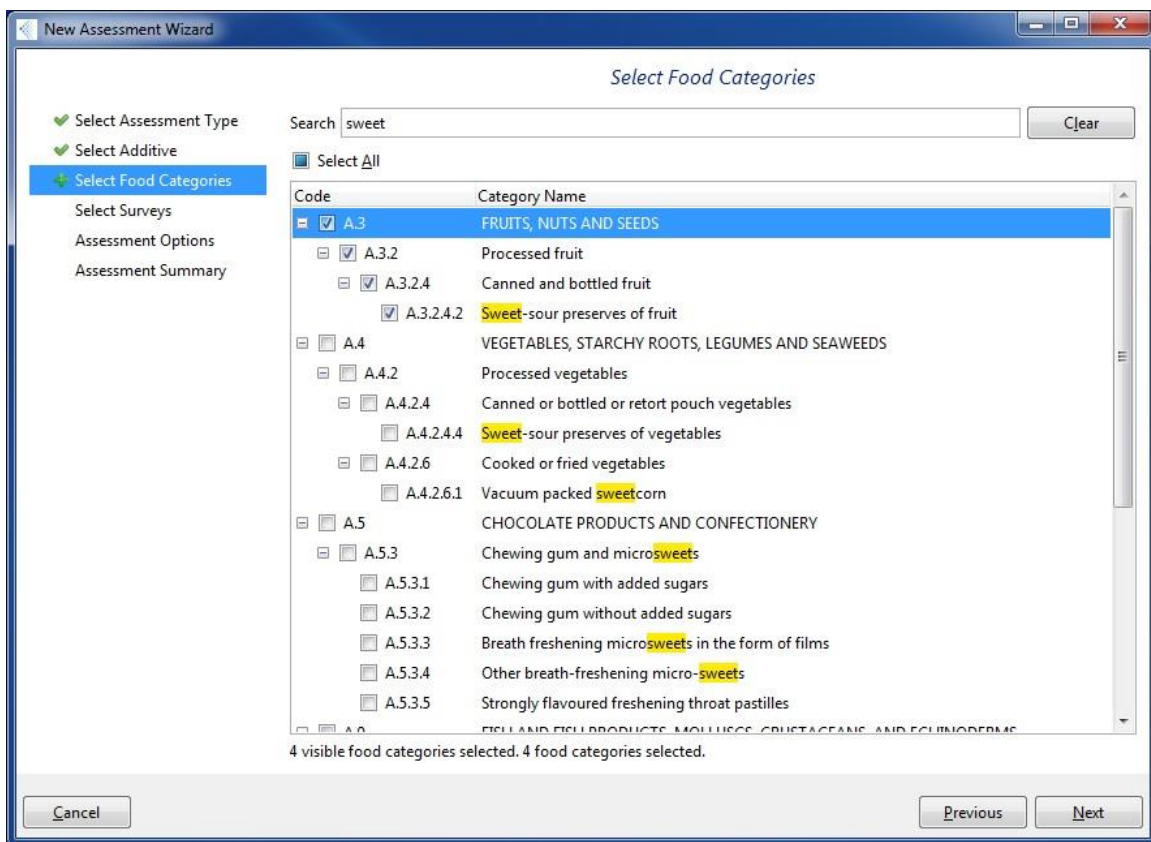


Figure 21: Searching for and selecting food categories

Select Survey

Here, specific food consumption survey options with which to perform assessments are presented to the user (Figure 22).

To choose a survey, simply click on one from the list and click on the “Next” button. Note that some countries have more than one survey. Multiple surveys can also be selected, and all surveys can be selected for use in an assessment by clicking the “Select All” checkbox in the top left hand corner of the view. Note that selecting all surveys for a particular assessment can take a long time to run.

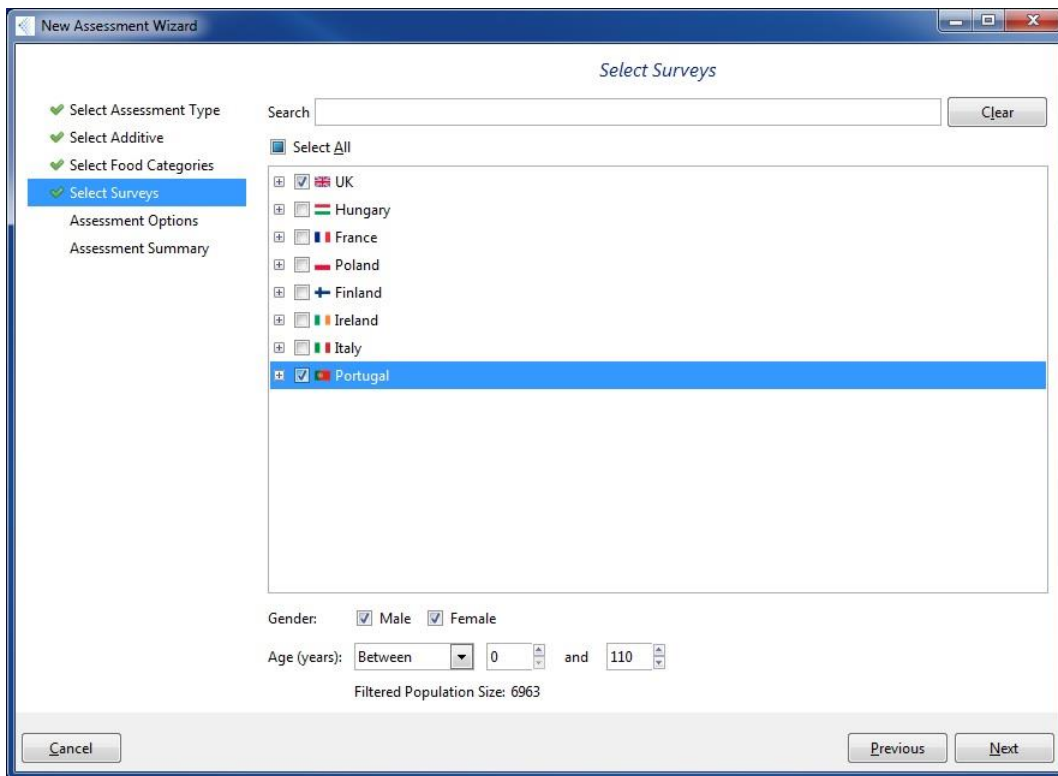


Figure 22: Selecting a survey

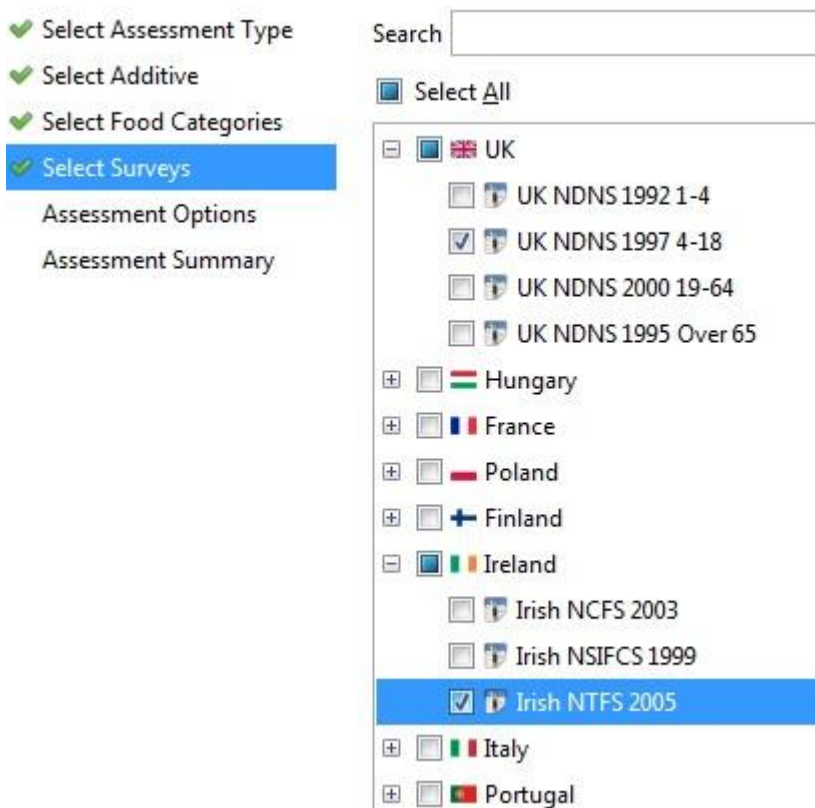


Figure 23: Example of country with multiple surveys and selecting two surveys to compare.

Select Population Filters

Here, sex and age population filters are available for refinement of the assessment. Selecting one or more of these filters allows users to perform an assessment on that subset of the population. The “All” option is selected by default, meaning both males and females are both included and all ages. To define age, the following options are available from the drop down menu:

- Between (specifying upper and lower limits, inclusively)
- Less than
- Greater than

The user can then enter numerical values relating to the filter chosen from the above list.



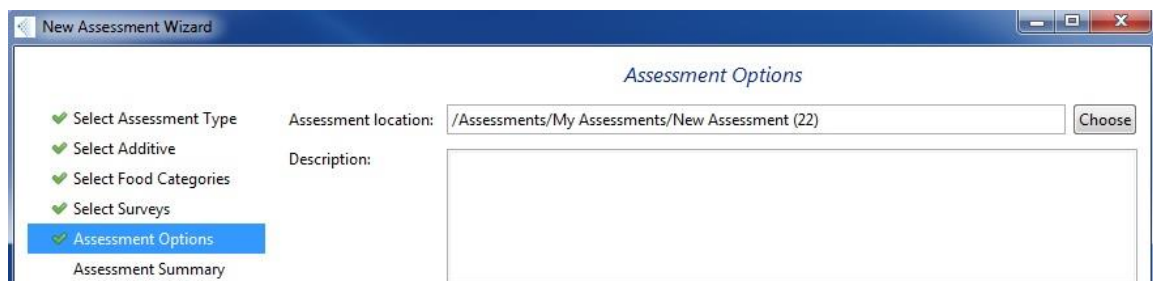
The screenshot shows a web interface for selecting population filters. Under the 'Gender' section, the 'Male' checkbox is checked, and the 'Female' checkbox is unchecked. Under the 'Age (years)' section, a dropdown menu is open, showing three options: 'Between', 'Less Than', and 'Greater Than'. The 'Between' option is selected, and the text 'Size: 1068' is displayed next to it. To the right of the dropdown, there are two input fields: the first contains '0' and the second contains '97', separated by the word 'and'. At the bottom right of the form, there are two buttons: 'Previous' and 'Next'.

Figure 24: Selecting population filters

Note that for an assessment involving multiple surveys, the age filters are applied across all surveys simultaneously, so some age bands may not apply to a given survey.

Assessment Options

In the basic view, the option of naming the assessment is given as well as providing a description of the assessment. Users can name assessments and choose a location for it in the Assessments tab by clicking on the “Choose” button (Figure 25). It is recommended that a sufficiently descriptive name is chosen in place of the default “New Assessment” title. In the “Assessment description” text box, the user can enter additional details about their assessment.



The screenshot shows a window titled 'New Assessment Wizard'. On the left side, there is a vertical list of steps, each with a green checkmark icon: 'Select Assessment Type', 'Select Additive', 'Select Food Categories', 'Select Surveys', and 'Assessment Options'. The 'Assessment Options' step is highlighted with a blue background. Below this list, the text 'Assessment Summary' is visible. On the right side of the window, the title 'Assessment Options' is displayed. Below the title, there are two fields: 'Assessment location:' with the text '/Assessments/My Assessments/New Assessment (22)' and a 'Choose' button to its right; and 'Description:' with a large, empty text area below it.

Figure 25: Basic view of assessment options.

An output folder for the assessment is chosen by clicking on the “Choose” button. This opens a pop up window, giving you the option of selecting a destination folder. By default, all

assessments are contained in the “Assessments” folder. A subfolder can be created by clicking on the “New Folder” button at the bottom of the dialogue box, and then entering a name for the new folder. Alternatively, users can right click on where they want to create a folder and select “New Folder” from the context menu.

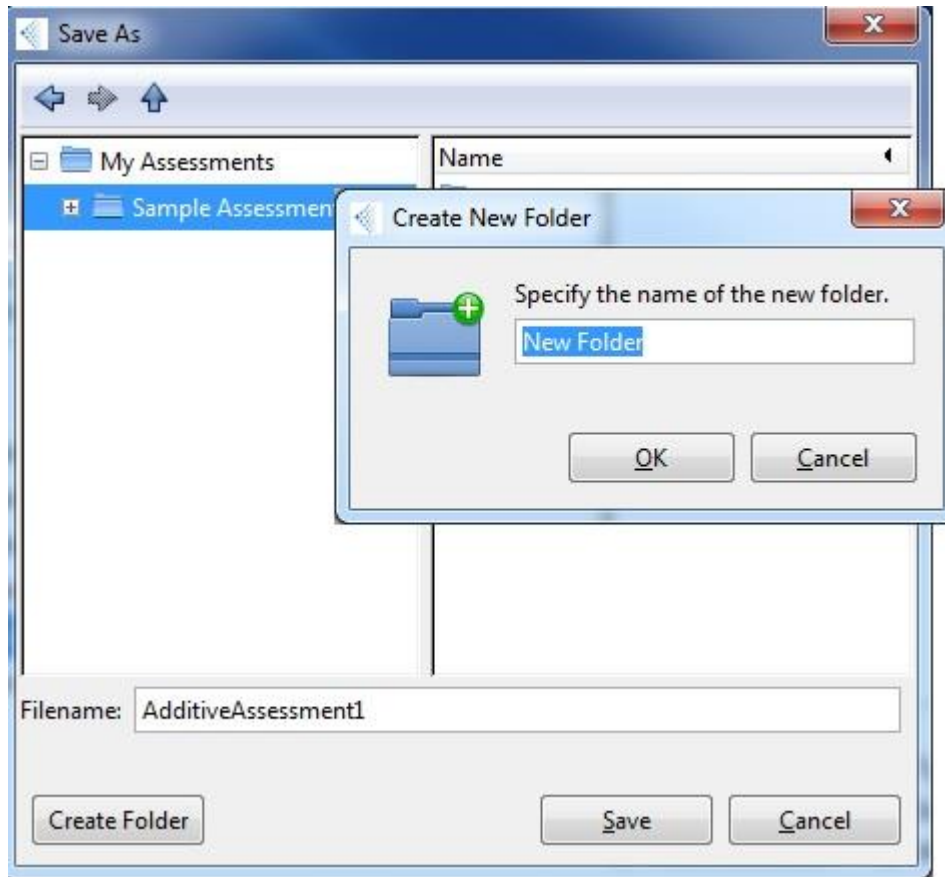


Figure 26: Choosing an output folder.

Flavouring Assessment Options

Depending on the substance and database chosen, there are a number of options for a flavouring assessment:

Assessment Options

Assessment Summary

Assess using:

☐ Typical use levels ☒ Upper use levels

☐ Fitted Distribution

Exclude foods without added flavourings: ☒

Exclude unprocessed fruits, nuts and seeds: ☐

Use probability of addition data: ☐

Flavouring source:

☒ Added and Natural ☐ Added Only ☐ Natural Only

+ Advanced Options

Cancel Previous Next

Figure 27: Flavouring options

Assess using: The exposure assessment can be performed using either:

- Typical use levels
- Upper use levels
- Fitted distribution (a parametric distribution fitted to the typical and upper use levels)

Exclude unflavoured foods: Consumption events described as being “without added flavourings” are ignored in the exposure assessment.

Exclude homemade foods: Consumption events described as being homemade are ignored in the exposure assessment.

Use probability of addition data: Use probability of addition data for flavourings that have this value assigned (only applies to the target flavourings in FACET).

Flavouring source: Assess exposure due to:

- Added and natural
- Added only
- Natural only

The option for assessing exposure due to natural occurrence only applies to the target flavourings in FACET.

Additive Assessment Options

Depending on the substance chosen, the user has a number of options for an additive assessment:

Assessment Options
Assessment Summary

Assess using:

- ☒ Typical Minimum
- ☐ Typical Maximum
- ☐ Extreme Minimum
- ☐ Extreme Maximum
- ☐ Fitted Distribution
- ☐ MPL

Include occurrence data: ☐

Advanced Options

Cancel Previous Next

Figure 28: Additive options.

Assess using: The exposure assessment can be performed using:

- Typical minimum concentrations
- Typical maximum concentrations
- Extreme minimum concentrations
- Extreme maximum concentrations
- Fitted distribution
- Maximum Permitted Levels (MPLs)

The first five options only apply to the 32 target additives and are based on data supplied by industry.

Packaging Assessment Options

Consumer loyalty: For a packaging assessment, users can choose to perform the assessment with, without, or both with and without consumer loyalty model (this appears in the advanced options for the other assessment types).

SetOff: If the substance in the assessment has been pre-populated with set-off then, at this point, the user has the option to run the assessment with set-off. Otherwise, the user will not be allowed to check the “Use SetOff” option.

Exclude homegrown/homemade foods: Consumption events described as involving homegrown foods are ignored.

Exclude restaurant/canteen foods: Consumption events described as involving restaurant or canteen foods are ignored.

Figure 29: Assessment Options

Advanced Options

If the “Show Advanced Options” option is clicked, additional options relating to the statistics of the assessment are made available for selection (Figure 30).

Advanced Options

Include lowest tier results: ☐

Minimum simulated population size: 1001

Exposure statistics:

<input checked="" type="checkbox"/> Mean	<input checked="" type="checkbox"/> Standard Deviation	<input checked="" type="checkbox"/> Minimum	<input checked="" type="checkbox"/> Maximum
<input checked="" type="checkbox"/> P25	<input type="checkbox"/> P50	<input type="checkbox"/> P75	<input checked="" type="checkbox"/> P90
<input checked="" type="checkbox"/> P95	<input type="checkbox"/> P97.5	<input type="checkbox"/> P99	<input type="checkbox"/> P99.9

Other percentiles:

Previous Next

Figure 30: Advanced Options

These are:

- **Include lowest tier results:** Include output for all food categories at the lowest tier. Note that this causes the assessment to take much longer to run.
- **Minimum simulated Population Size:** This is a numeric field, allows the user to change the size of the population used in the simulation. The number specified is the minimum population size used in the assessment; the actual number used will be increased to the next multiple of the number of subjects chosen after the filtering in Step 7.
- **Exposure Statistics:** These are checkboxes that allow the user to include the following statistics in the assessment (the first four options, P90, and P97.5 are selected by default):
 - Mean
 - Standard Deviation
 - Minimum
 - Maximum
 - P25
 - P50
 - P75
 - P90
 - P95
 - P97.5
 - P99
 - P99.9
- **Other Percentiles:** This is a numeric field. Other percentiles can be entered, separated by commas (e.g. 92, 93).

- **Confidence Intervals:** These are checkboxes that allow the user to specify the following confidence intervals (the standard error is selected by default):
 - Standard Error
 - 90% Confidence Interval
 - 95% Confidence Interval
 - 99% Confidence Interval
- **Other Confidence Intervals:** This is a numeric field. Other confidence intervals can be entered, separated by commas (e.g. 75, 85).
- **Use consumer loyalty:** For additives and flavourings, a consumer loyalty model can be used as part of the exposure assessment. This brings up a new set of food categories to used in the consumer loyalty model.
- **Truncate at SML value:** This only applies to packaging assessments. If chosen, an SML can be entered to truncate concentration values calculated by the migration model.

Assessment Summary

This step presents a summary of the current choices of substances, populations and food categories for the assessment.

After reviewing the choices, users can choose to start an assessment using the “Run” button at the bottom right of the window. At the bottom of the summary the estimated time for the assessment to run is shown. In order to start the assessment, the check box must be ticked indicating an understanding that your computer will be busy for the time taken to run the assessment.

Changes can be made to the selections before the assessment is submitted. Navigation to the appropriate steps to do this is easily achieved with the buttons on the left of the tab.

Renaming an Assessment

1. To rename an assessment, right click on the assessment to delete and select “Rename” from the context menu.
2. Alternatively, select the assessment to rename and choose “Rename” from the Edit menu.

Deleting an Assessment

1. To delete an assessment, right click on the assessment and select “Delete” from the context menu.
2. Alternatively, select the assessment and choose “Delete” from the Edit menu.
3. Note that if the assessment is not yet complete, users can still delete it.

Viewing the Results Report

To view the report generated by the software:

1. Navigate to where the assessment is located in the assessment manager and click on it.
2. A summary of the assessment will appear in the bottom right pane.
3. Click on the “View report” button in the top right hand side of the preview pane. This will bring up the report viewer, showing a summary of the report and some basic statistics.
4. To print the report, click on the “Print” button in the top right left hand corner of the report.
5. To save the report in PDF format, click on the “Export” button in the top left hand corner of the report.

Viewing Graphs of the Assessment Results

To view graphs and statistics generated by an assessment:

1. Navigate to where the assessment is located in the assessment manager and click on it.
2. A summary of the assessment will appear in the bottom right pane.
3. Click on the “View Graphs” button in the top right hand side of the preview pane. This will bring up the results viewer, showing graphs and statistics generated by the assessment.

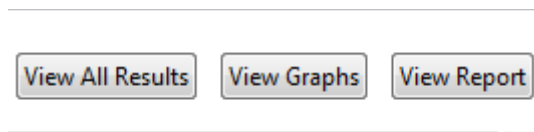


Figure 31: View results buttons

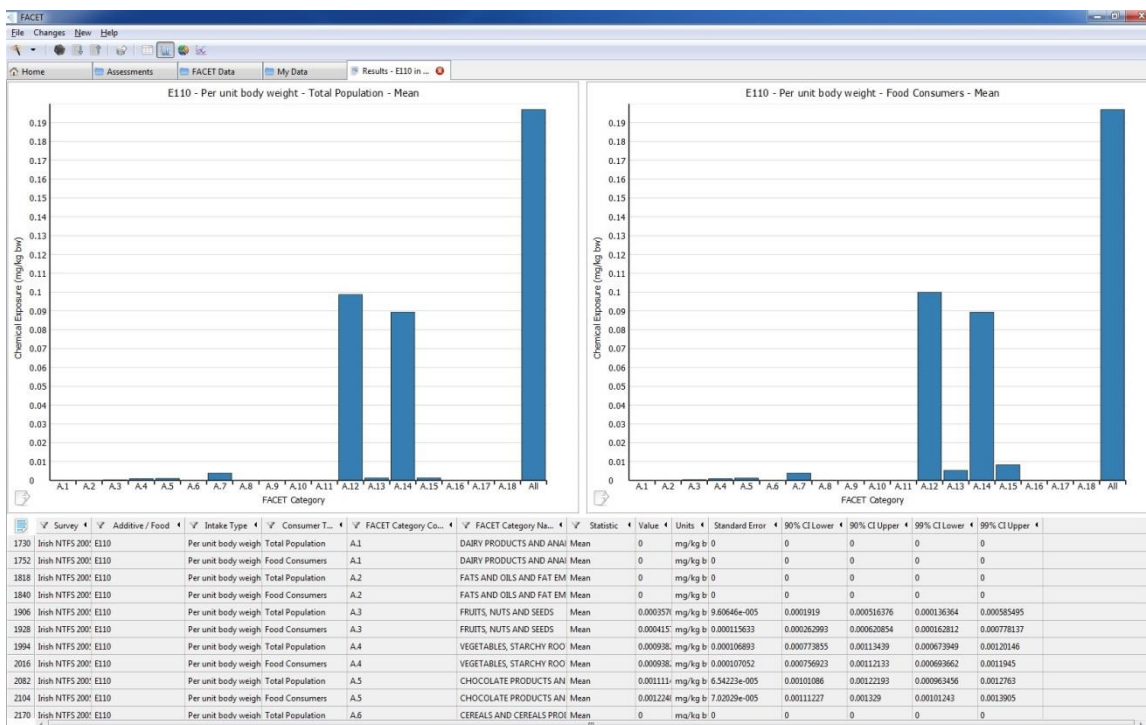


Figure 32: Results viewer –Column Chart and Data

There are four available views, three graphical views (column charts, pie charts, and distributions) and a data view. To toggle between the views click on the different graph icons or the data icon in the toolbar.

Viewing Graphs

By default, the assessment results appear with graphical views of the exposure assessments are presented above the data grid. The content of the graphs is controlled by the filters on the data grid fields.

To control the type of graph being displayed, click on the different graph icons in the tool bar. There are three graph types:



Column Chart: A chart with vertical rectangular bars with lengths proportional to the values that they represent. The level of exposure is on the y-axis and the FACET food category is on the x-axis (Figure 32).



Pie chart: A circular chart divided into sectors, illustrating proportion. The arc length of each sector is proportional to the quantity it represents. The chart is displayed with a legend on the right hand side, and only applies to the mean statistic in the total population (Figure 10).

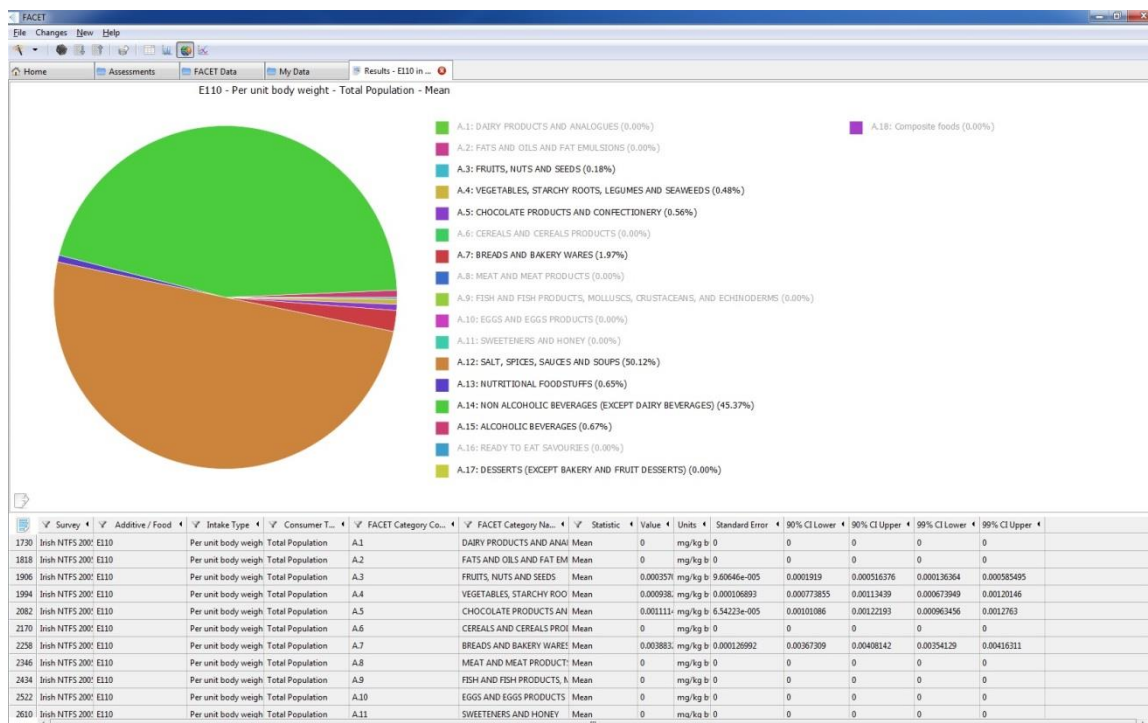


Figure 33: Results viewer – Pie Chart and Data



Distribution: There are two types of distribution charts, which can be selected from the “statistic” column in the data grid.

- **PDF:** Probability density function, which describes the relative likelihood for a random variable to occur at a given point (note that in cases when there is a constant amount of exposure for all subjects the range of the PDF will be 0 to 1e-06, purely for graphing purposes).
- **CDF:** Cumulative distribution function, which displays the probability that an exposure value will be found at a value less than or equal to a given number (Figure 34).

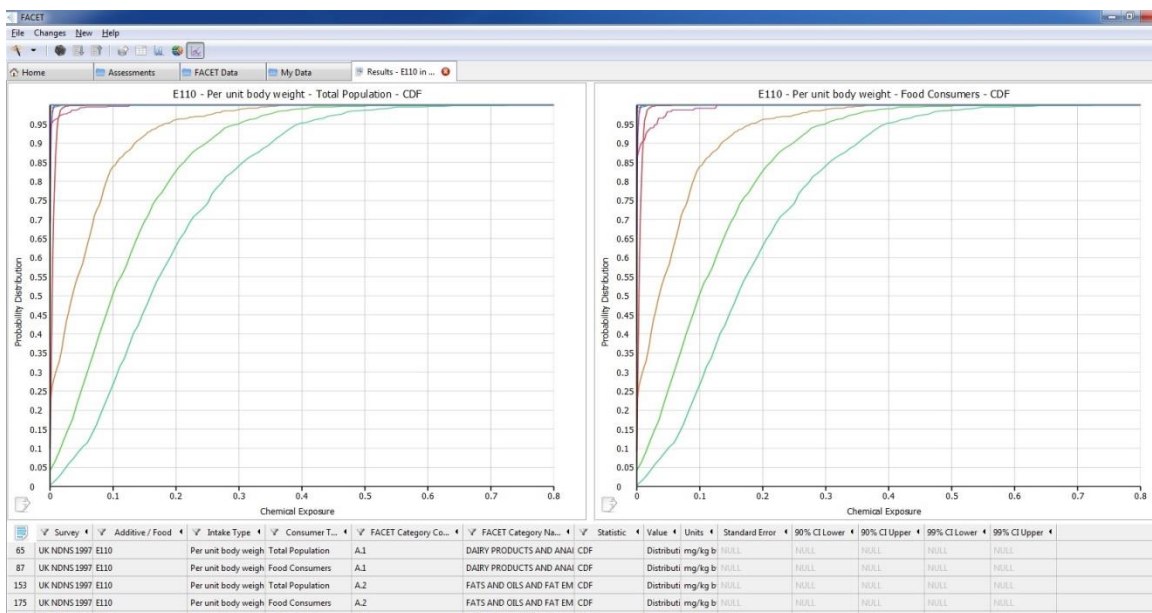


Figure 34: Results viewer: Line Graph and Data

To control what data appears on a selected graph there are filters in the headers of each column (Figure 35). Clicking on the header shows the available filters for that field. There are two filter types:

	Survey	Additive / Food	Intake Type	Consumer T...	FACET Category Co...	FACET Category Na...	Statistic	Value	Units	Standard Error
1730	Irish NTFS 2000	E110	Per unit body weight	Total Population	A.1	DAIRY PRODUCTS AND ANAI	Mean	0	mg/kg bw	0
1818	Irish NTFS 2000	E110	Per unit body weight	Total Population	A.2	FATS AND OILS AND FAT EM	Mean	0	mg/kg bw	0
1906	Irish NTFS 2000	E110	Per unit body weight	Total Population	A.3	FRUITS, NUTS AND SEEDS	Mean	0.000357	mg/kg bw	9.60646e-005
1994	Irish NTFS 2000	E110	Per unit body weight	Total Population	A.4	VEGETABLES, STARCHY ROO	Mean	0.000938	mg/kg bw	0.000106893
2082	Irish NTFS 2000	E110	Per unit body weight	Total Population	A.5	CHOCOLATE PRODUCTS AN	Mean	0.001111	mg/kg bw	6.54223e-005
2170	Irish NTFS 2000	E110	Per unit body weight	Total Population	A.6	CEREALS AND CEREALS PROI	Mean	0	mg/kg bw	0
2258	Irish NTFS 2000	E110	Per unit body weight	Total Population	A.7	BREADS AND BAKERY WARES	Mean	0.003883	mg/kg bw	0.000126992
2346	Irish NTFS 2000	E110	Per unit body weight	Total Population	A.8	MEAT AND MEAT PRODUCT	Mean	0	mg/kg bw	0
2434	Irish NTFS 2000	E110	Per unit body weight	Total Population	A.9	FISH AND FISH PRODUCTS, N	Mean	0	mg/kg bw	0
2522	Irish NTFS 2000	E110	Per unit body weight	Total Population	A.10	EGGS AND EGGS PRODUCTS	Mean	0	mg/kg bw	0
2610	Irish NTFS 2000	E110	Per unit body weight	Total Population	A.11	SWEETENERS AND HONEY	Mean	0	mg/kg bw	0

Figure 35: Filters available.

- **Checkboxes:** This filter type applies to data that can be plotted simultaneously (e.g. *FACET category codes* in Figure 35 which relate to Foods).
- **Radio Buttons:** This filter type applies to data that cannot be plotted simultaneously (e.g. the *Statistic* column in Figure 35).

Each filter type is described in detail below:

- **Survey:** Used to alternate between different dietary surveys in an exposure assessment. This has a radio button type filter.
- **Substance/Food:** Used to alternate between displaying exposure to a substance or intake of food. This has a radio button type filter.
- **Intake Type:** The type of exposure, which can be “Absolute” (measured in mg per day) or “Per unit body weight” (measured in mg per kilogram of bodyweight per day). This has a radio button type filter.

- **Consumer Type:** There are two possible consumer types, “Food Consumers” and “Total Population”. As these cannot be plotted together, each consumer type appears in a separate graph. This has a checkbox type filter.
- **FACET Category Code:** This allows users to decide which FACET food categories are displayed, by their numerical food code. This has a checkbox type filter.
- **FACET Category Name:** This allows users to decide which FACET food categories are displayed, by their food description. This has a checkbox type filter.
- **Statistic:** Shows what population statistic is plotted (e.g. mean, P90, P95 etc). This has a radio button type filter. When a distribution chart type is selected, this filter provides the option of displaying a PDF or CDF chart type.

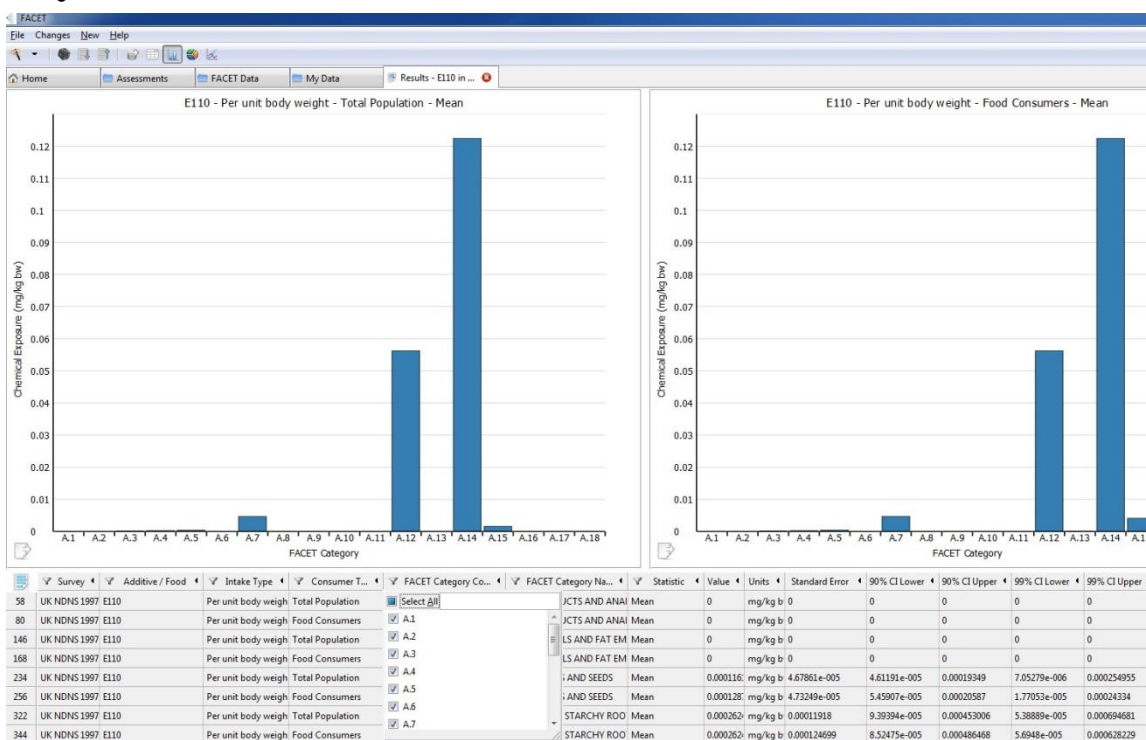


Figure 36: Column chart and data

There are additional fields that are used to display values in the chart type. These are:

- **Value:** The numerical value(s) of exposure being displayed and plotted, according to the filter settings chosen.
- **Units:** The units of the numerical value being displayed.
- **Standard Error and Confidence Intervals:** These are used to display any confidence intervals calculated for the assessment, presented as upper and lower bounds. In the case of the standard error, this is a single value.

The values displayed can be exported as a CSV (Comma-Separated Values) file at any time by clicking on the export data icon located in the toolbar:



Data exported in CSV formatted can be opened later in a spreadsheet program including Microsoft Excel.

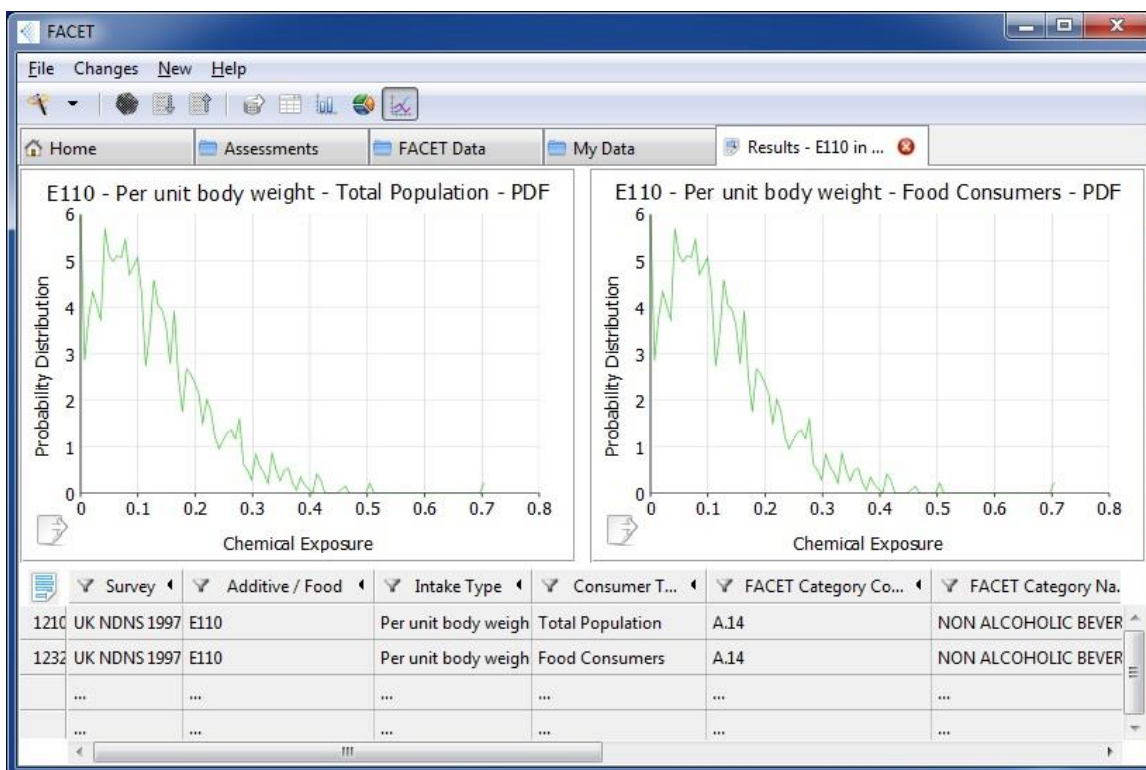


Figure 37: Probability density function chart and data

Viewing Data Only

To see the raw data calculated in an exposure assessment, click on the table icon in the toolbar. This will bring up a data-only view:



The table fields are the same as before, when the different graphs are being shown. However, since all the data is no longer being plotted, different combinations of data can be viewed simultaneously. Thus, all the filters are checkboxes when this view is selected.

The values displayed can be exported as a CSV (Comma-Separated Values) file at any time by clicking on the export icon located in the top left hand corner of the data grid:



Data exported in CSV formatted can be opened later in a spreadsheet program including Microsoft Excel.

	FACET Category Co...	FACET Category Na...	Statistic	Value	Units	Standard Error	90% CI Lower
1	A.1	DAIRY PRODUCTS AND ANA...	Count	1206		0	
2	A.1	DAIRY PRODUCTS AND ANA...	Percentage Consu...	100	%	0	
3	A.1	DAIRY PRODUCTS AND ANA...	Mean	214.835	g	4.23178	
4	A.1	DAIRY PRODUCTS AND ANA...	Standard Deviatio...	155.209	g	4.30623	
5	A.1	DAIRY PRODUCTS AND ANA...	Minimum	0	g	0.209841	
6	A.1	DAIRY PRODUCTS AND ANA...	Maximum	871.588	g	18.7314	
7	A.1	DAIRY PRODUCTS AND ANA...	P25	101.997	g	4.89288	
8	A.1	DAIRY PRODUCTS AND ANA...	P90	429.841	g	13.4244	
9	A.1	DAIRY PRODUCTS AND ANA...	P97.5	617.781	g	21.4082	
10	A.1	DAIRY PRODUCTS AND ANA...	CDF	Distributi...	g	NULL	
11	A.1	DAIRY PRODUCTS AND ANA...	PDF	Distributi...	g	NULL	
12	A.1	DAIRY PRODUCTS AND ANA...	Count	1206		0	
13	A.1	DAIRY PRODUCTS AND ANA...	Percentage Consu...	100	%	0	
14	A.1	DAIRY PRODUCTS AND ANA...	Mean	0	mg	0	
15	A.1	DAIRY PRODUCTS AND ANA...	Standard Deviatio...	0	mg	0	

Figure 38: Data only view

Viewing All Results

Results can be viewed in all food categories at the lowest, if this option is selected when the assessment is run (see “Running an Assessment” for details). If this option is checked when the assessment is run the button “View All Results” will be available. If this option is not chosen when the user ran the assessment, this option will be greyed out. To view results generated by an assessment:

1. Navigate to where the assessment is located in the assessment manager and click on it.
2. A summary of the assessment will appear in the bottom right pane.
3. Click on the “View All Results” button in the top right hand side of the preview pane (if available). This will bring up the results viewer, showing all statistics generated by the assessment at all food groups.

The results are outputted as a table that can be filtered as desired. Any result can be viewed simultaneously, so all fields have checkbox type filters. Each filter type is described in detail below:

- **Survey:** Used to alternate between different dietary surveys in an exposure assessment.
- **Substance/Food:** Used to alternate between displaying exposure to a substance or intake of food.
- **Intake Type:** The type of exposure, which can be “Absolute” (measured in mg per day) or “Per unit body weight” (measured in mg per kilogram of bodyweight per day).
- **Consumer Type:** There are two possible consumer types, “Food Consumers” and “Total Population”.
- **FACET Food Code:** This allows users to decide which FACET food categories are displayed, by their numerical food code.
- **FACET Food Name:** This allows users to decide which FACET food categories are displayed, by their food description.
- **Statistic:** Shows what population statistic is plotted (e.g. mean, P90, P95 etc).

7. FACET Data

The FACET data tab allows users to view (but not edit) FACET data used in performing exposure assessments. Note that raw concentration data, packaging data, and consumption diaries will be hidden from the user at all times.

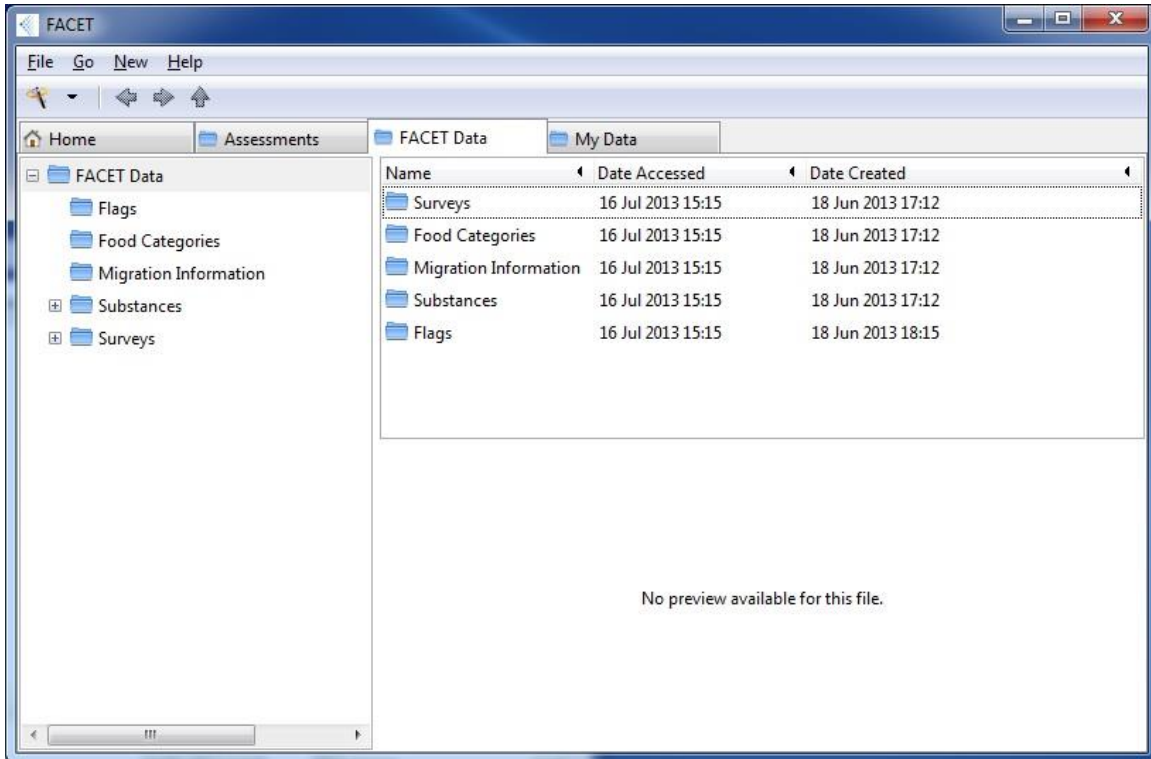


Figure 39: The FACET Data Tab

The tab is implemented in a three pane layout. The upper pane contains folders of data tables that can be selected and viewed, and left-hand pane shows a tree structure that shows how the FACET folders are organised. The bottom pane displays the contents of certain tables in the upper pane.

There are six main folders:

- Flags
- Food Categories
- Migration Information
- Substances
- Surveys

Clicking on the plus symbol next to each folder in the folder tree causes the contents of the tree to expand. Each folder is described in detail below

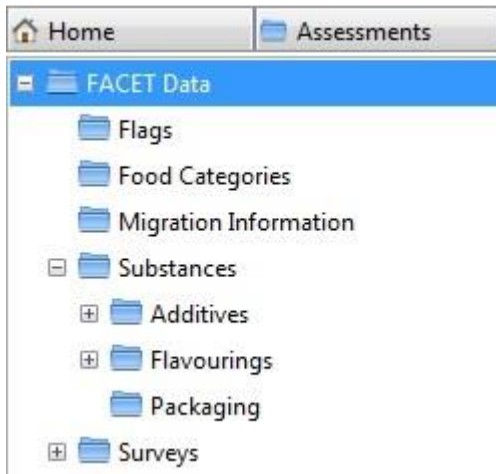


Figure 40: Expanding folders using the plus symbol.

Flags

This folder contains tables of the different possible flags used in the consumption diaries and chemical concentration tables. Flags with the same meaning and settings are grouped in the same tables. Both the numerical value and the text description of the flag settings are given in each table.

Food Categories

This folder provides a list of all food categories in FACET. The food categories are hierarchical, and there is a separate system for flavourings, additives and packaging. There are three systems:

- Additives Food Hierarchy
- Flavourings Food Hierarchy
- Packaging Food Hierarchy

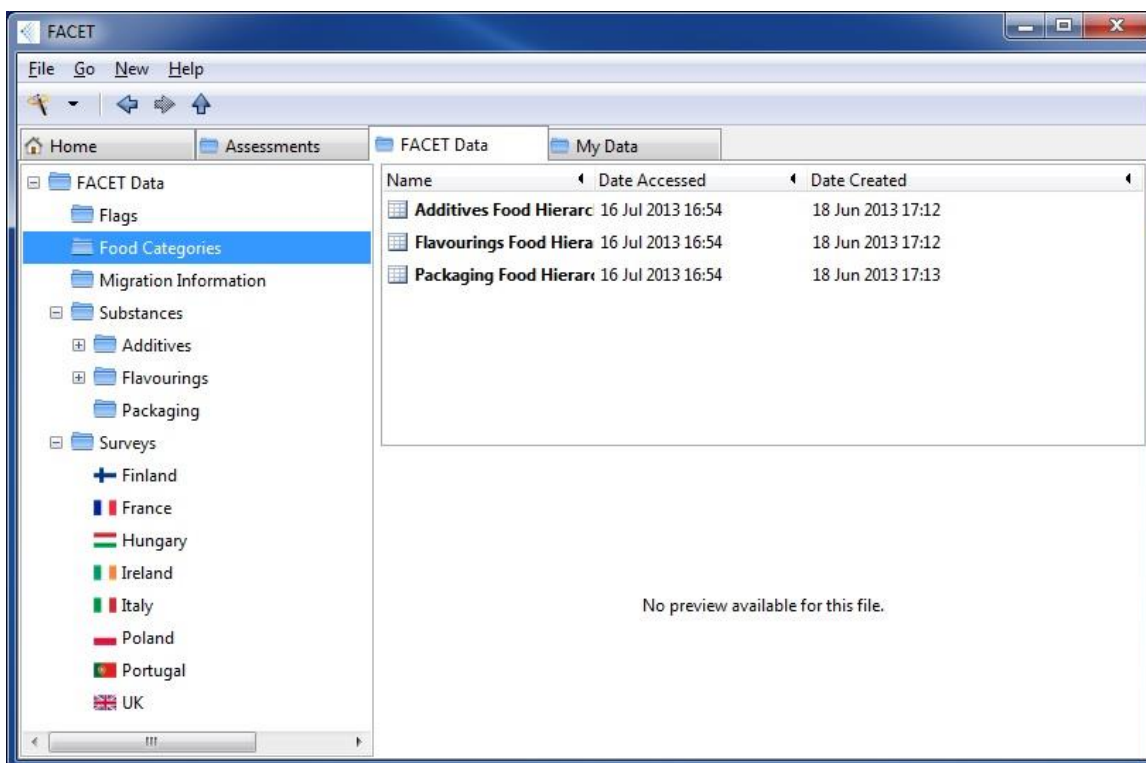


Figure 41: Food Categories Folder.

Clicking on each table causes it to appear in the pane below. The fields in each table are:

- Category Code
- Category Name

FACET Data		My Data	
Name	Date Accessed	Date Created	
Additives Food Hierarc	16 Jul 2013 16:54	18 Jun 2013 17:12	
Flavourings Food Hiera	16 Jul 2013 16:54	18 Jun 2013 17:12	
Packaging Food Hierarc	16 Jul 2013 16:54	18 Jun 2013 17:13	

Search

Code	Category Name
+ F.1	Dairy products and analogues including ingredients of composite foods
+ F.2	Fats and oils and fat emulsions including ingredients of composite foods
+ F.3	Fruits, nuts and seeds including ingredients of composite foods
+ F.4	Vegetables, starchy roots, legumes and seaweeds including ingredients of composite f...
+ F.5	Chocolate products and confectionery including ingredients of composite foods
+ F.6	Cereals and cereal products including ingredients of composite foods
+ F.7	Breads and bakery wares including ingredients of composite foods
+ F.8	Meat and meat products including ingredients of composite foods

Figure 42: Fields available in each table.

Each system can be viewed as a tree, and clicking on the arrow in each category causes the contents of that category to be displayed, which in turn can be expanded and so on. The data can also be searched using the search box that appears between the panes.

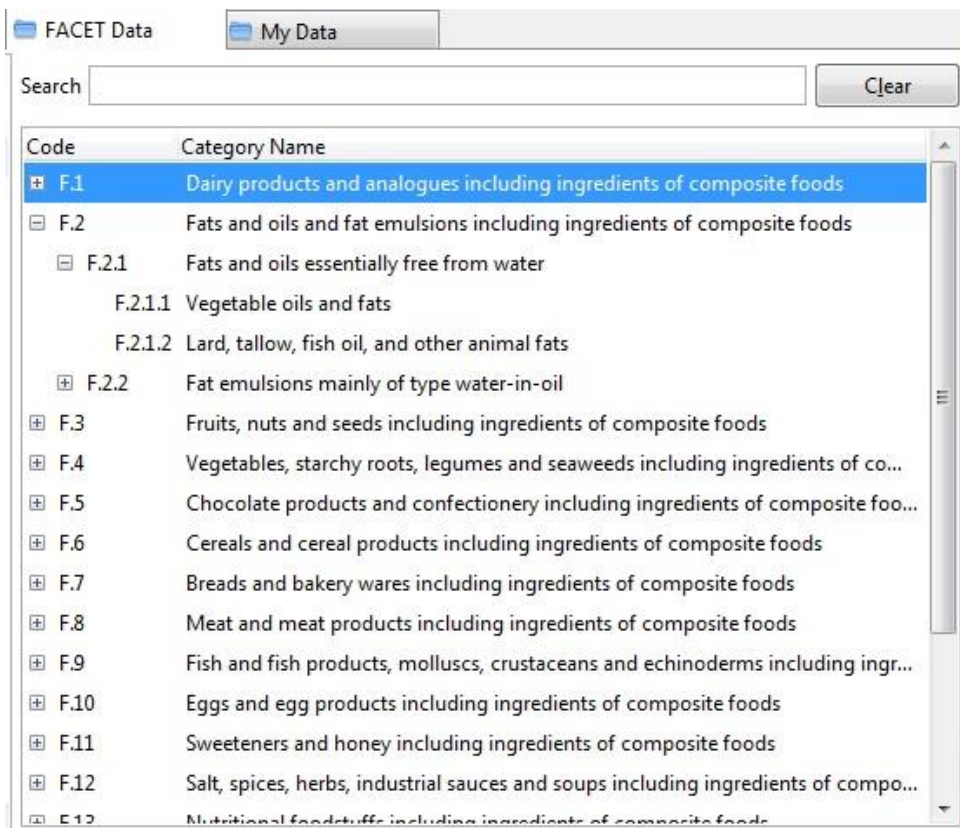


Figure 43: Example of category tree.

Migration Information

This folder contains all material codes and pack types used in FACET.

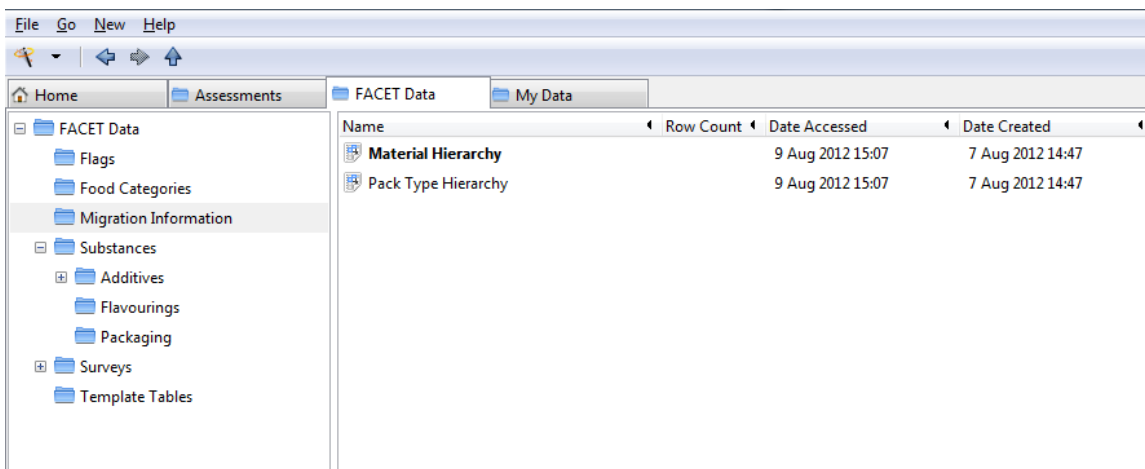


Figure 44: Material Code folder.

The fields in the Material Hierarchy table are:

- Material Code
- Material Name

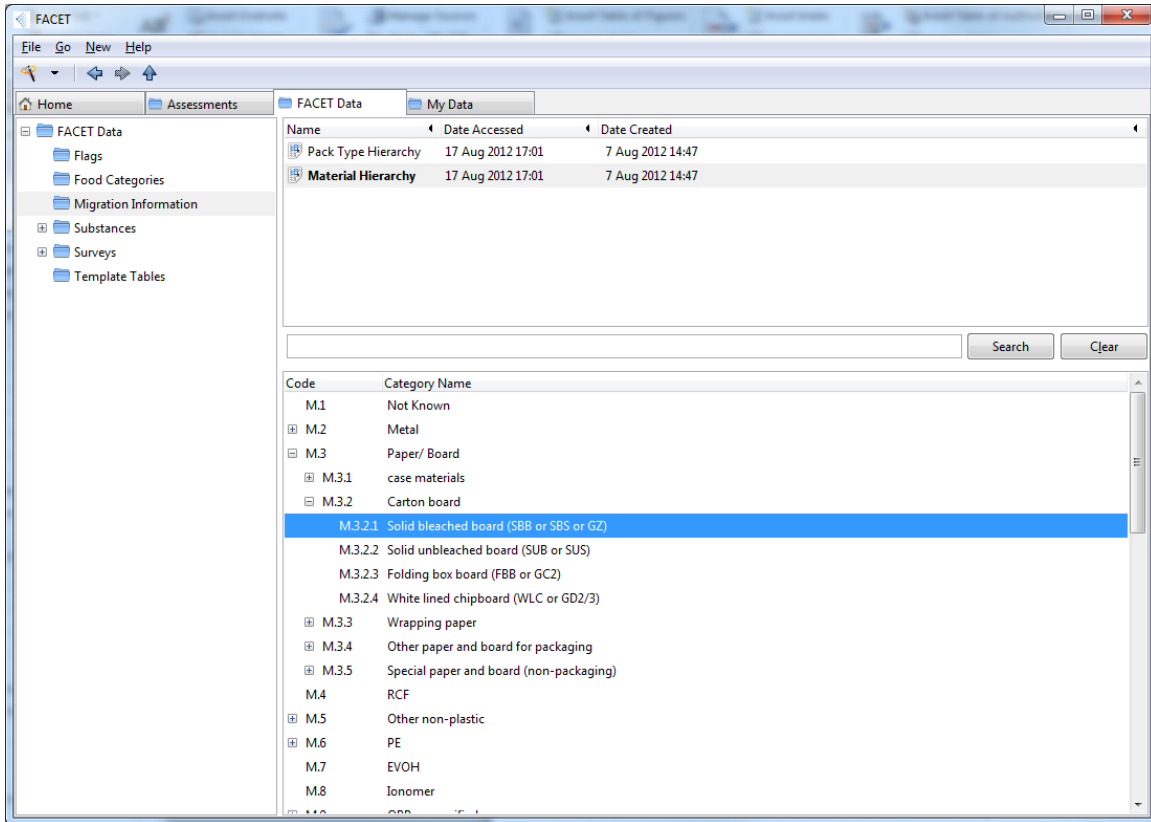


Figure 45: Material Code Table

The material codes can be viewed as a tree, and clicking on the arrow in each category causes the contents of that category to be displayed, which in turn can be displayed. The data can also be searched using the search box that appears between the panes.

The Pack Type Hierarchy table shows the pack type descriptions contained in the Main, Closure, Outer, and Insert components of food packaging. It is in a hierarchy in the same form as the Material Hierarchy table.

Substances

This view provides a list of all substances in FACET. There are three folders, each of which is described in detail below. Double-clicking on any of the tables will open a data view of that table for so that the content can be browsed easily.

Name	Date Accessed	Date Created
Additives	Feb 28 09:10	Feb 27 12:37
Flavourings	Feb 28 09:10	Feb 27 12:37
Packaging	Feb 28 09:10	Feb 27 12:37

Figure 46: Substances folders.

Flavourings

The flavourings folder contains tables of all of the flavourings data in FACET. There are two subfolders; the Flavouring Info folder and the Screening Calculations folder.

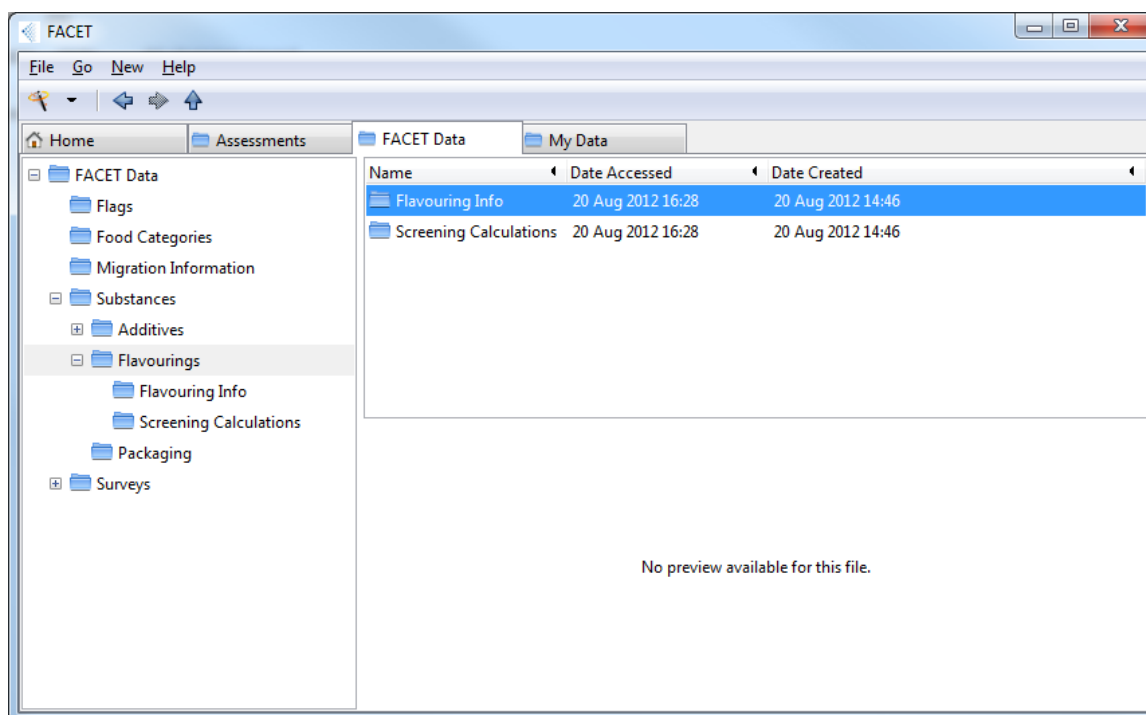


Figure 47: Flavourings folder

Flavourings Info

This folder contains tables detailing all the information on flavouring concentrations and other information.

The flavourings table (simply called “Flavourings”) contains information on all the different flavouring substances in FACET. Clicking on the table once will bring up a preview in the bottom right pane, showing a search box for browsing different fields. The table contains the following fields:

The screenshot shows a search interface for flavouring data. At the top, there is a search bar and a dropdown menu currently set to 'Flavis Number'. Below the dropdown, a list of search options is visible: 'Flavis Number', 'Name(s)', 'CAS Number', 'CoE Number', 'FEMA Number', and 'JECFA Number'. To the right of the dropdown are 'Search' and 'Clear' buttons. Below the search options is a table with the following data:

FI No	Flavis Name	CoE No	FEMA No	Jecfa N	T
2015	Menthol	63		427	N
2016	Borneol	64	2157	1385	N
2017	Cinnamyl alcohol	65	2294	647	N
2018	Nerolidol	67	2772		N
2019	2-Phenylethan-1-ol	68	2858	987	N
2020	Hex-2-en-1-ol	69	2562	1354	N

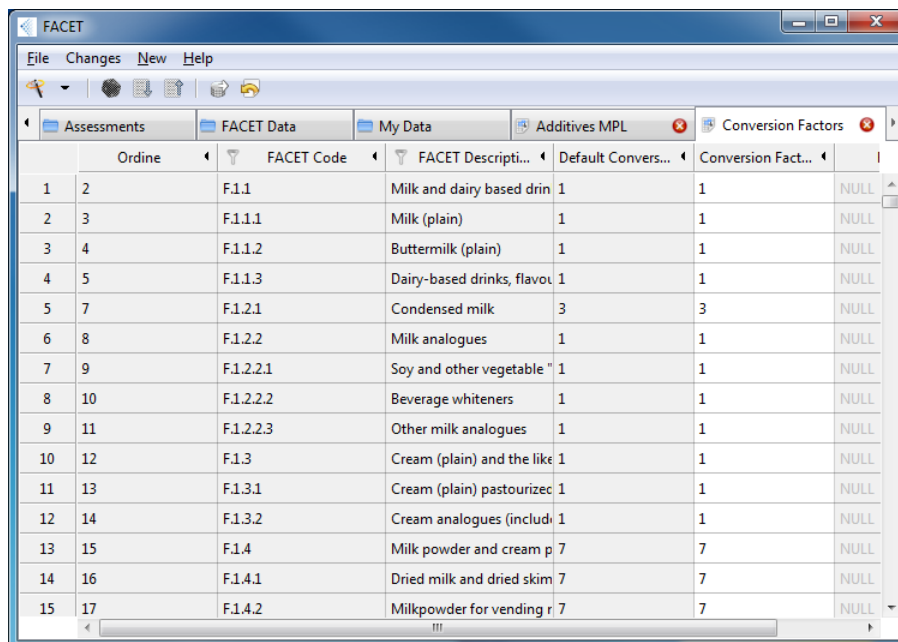
Figure 48: Search options for flavouring data.

- **Flavis Number:** Numeric field, the number assigned by FLAVIS – the EU Flavour Information System.
- **Flavis Name:** The name assigned by FLAVIS – the EU Flavour Information System.
- **CAS Number:** Chemical Abstracts Service. This is strictly of the form [up to 7 digits]-[2 digits]-[1 digit], e.g. “64-17-5”, or “0000064-17-5”.
- **CoE Number:** Council of Europe Number. This is strictly a numeric field, but can be any length.
- **FEMA Number:** Flavour and Extract Manufacturers Association. This is strictly a numeric field, but can be any length.
- **JECFA Number:** Joint FAO/WHO Expert Committee on Food Additives. This is strictly a numeric field, but can be any length.
- **Target Flavouring:** Yes/No field.
- **In Register:** Yes/No field.
- **Evaluation Status:** Whether evaluated or not and by whom.
- **Short Reference:** Reference to when the flavouring was assessed.
- **Synonymous:** Any synonyms for the flavouring.
- **Remarks:** Any further information about the flavouring.

There are 15 other tables in this folder:

- **Flavourings Refined:** The probability of addition of the target flavourings in difference FACET food categories, and refined use levels where known.
- **Flavourings EFFA:** Upper and average use levels from the European Flavour Association, in both the FACET and EFFA food categories.
- **Flavourings FEMA:** Upper and average use levels from the Flavour and Extract Manufacturers Association, in both the FACET and FEMA food categories.
- **Flavourings IOFI JECFA 2006:** Flavouring concentration database.
- **Flavourings IOFI JECFA 2007:** Flavouring concentration database.
- **Flavourings IOFI JECFA 2010:** Flavouring concentration database.
- **Flavourings IOFI:** Flavouring concentration database.
- **Flavourings DGSanco:** Flavouring concentration database.
- **Flavourings CoE:** Flavouring concentration database.
- **Flavourings Smoke:** Flavouring concentration database.
- **Conversion Factors:** Table of conversion factors for different food combinations.
- **Flavourings Natural Flag Setting:** For a given flag, shows for what foods with that flag setting are used to calculate a concentration value.
- **Flavourings Natural Food Categories:** What food categories can occur as recipe fractions.
- **Flavourings Natural Recipe Data:** What flags can occur as ingredient fractions.
- **Flavourings Natural:** Flavouring concentration database.

The Conversion Factors table can be modified to assess the impact of changing different conversion factors. The field that can be edited is in white. In order to restore the default values, click the “Restore Default” icon in the tool bar.



	Ordine	FACET Code	FACET Description	Default Conversion Factor	Conversion Factor
1	2	F.1.1	Milk and dairy based drinks	1	1
2	3	F.1.1.1	Milk (plain)	1	1
3	4	F.1.1.2	Buttermilk (plain)	1	1
4	5	F.1.1.3	Dairy-based drinks, flavoured	1	1
5	7	F.1.2.1	Condensed milk	3	3
6	8	F.1.2.2	Milk analogues	1	1
7	9	F.1.2.2.1	Soy and other vegetable protein	1	1
8	10	F.1.2.2.2	Beverage whiteners	1	1
9	11	F.1.2.2.3	Other milk analogues	1	1
10	12	F.1.3	Cream (plain) and the like	1	1
11	13	F.1.3.1	Cream (plain) pasteurized	1	1
12	14	F.1.3.2	Cream analogues (including	1	1
13	15	F.1.4	Milk powder and cream powder	7	7
14	16	F.1.4.1	Dried milk and dried skim milk	7	7
15	17	F.1.4.2	Milk powder for vending machines	7	7

Figure 49: Conversion Factors Table



Figure 50: Restore Default Icon

Screening Calculations

This folders contains tables of screening calculations for the different databases, namely the APET, SPET, TAMDI, and mTAMDI methods.

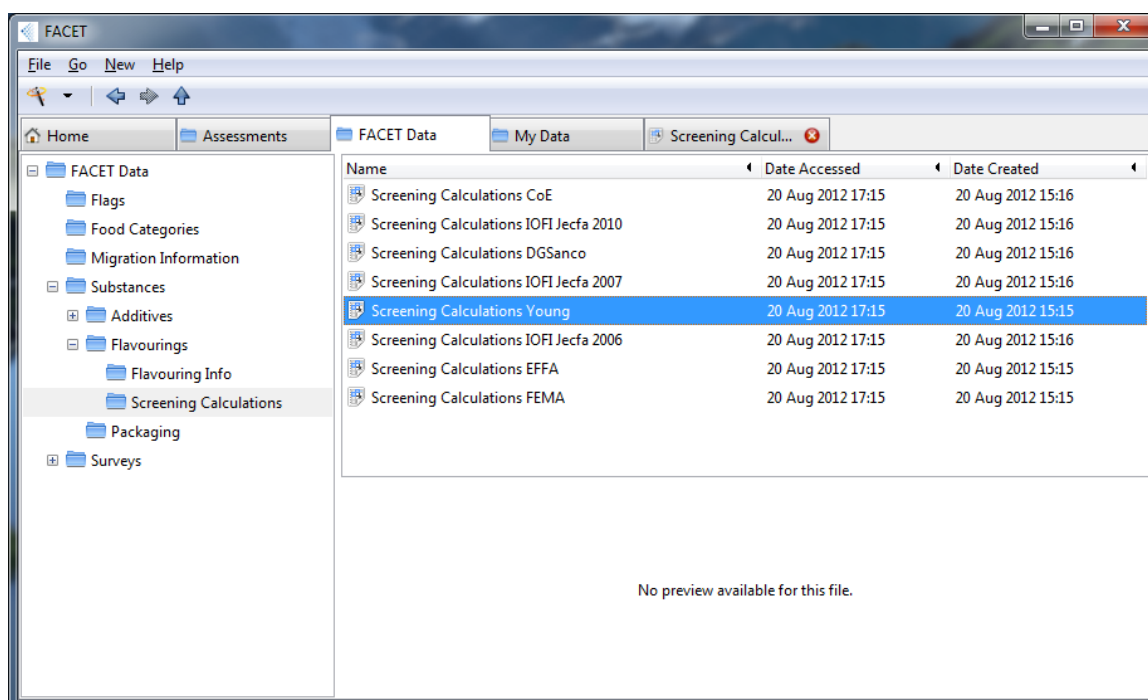


Figure 51: Screening Calculations Folder

Additives

The additive folder contains two subfolders; “Additive Info” and “Additive Ingredient Distributions”.

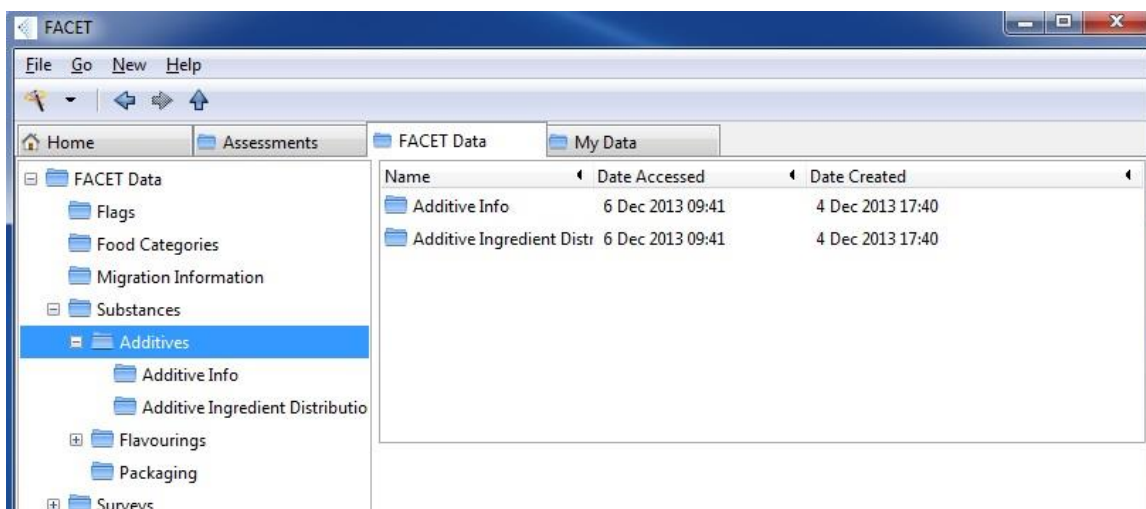


Figure 52: Additive Folder

Additive Info

The additive info folder contains three tables.

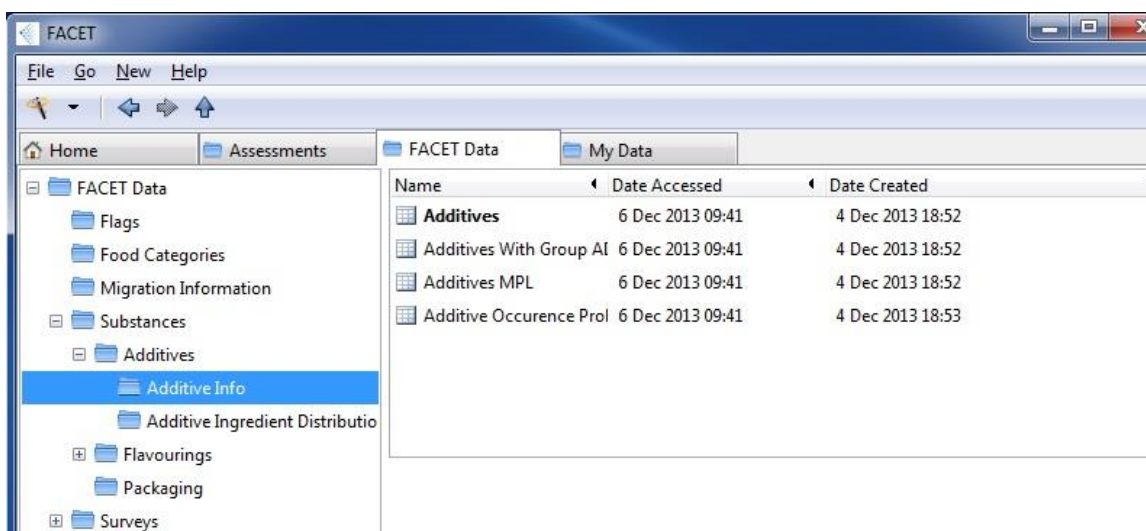


Figure 53: Additive Info Folder.

Additives MPL: A table of Maximum Permitted Levels (MPLs) for the FACET food categories and flag settings, as well as the calculated probability of addition.

The MPL values in this table can be changed, in order to assess the impact of varying the MPL values in an exposure assessment. The field that can be edited is in white. In order to restore the default MPLs, click the “Restore Default” icon in the tool bar.

	Additive Tier 1	FACET Code	FACET Description	Eu Code	Additive Name	Default Maxim...	Maximum Perm...
1	NULL	A.1.1.1.1	Sterilised and UHT milk	E338	Phosphoric acid	1000.0	1000
2	NULL	A.1.1.1.1	Sterilised and UHT milk	E339	Sodium phosphates	1000.0	1000
3	NULL	A.1.1.1.1	Sterilised and UHT milk	E340	Potassium phosphates	1000.0	1000
4	NULL	A.1.1.1.1	Sterilised and UHT milk	E341	Calcium phosphates	1000.0	1000
5	NULL	A.1.1.1.1	Sterilised and UHT milk	E343	Magnesium phosphates	1000.0	1000
6	NULL	A.1.1.1.1	Sterilised and UHT milk	E450	Diphosphates	1000.0	1000
7	NULL	A.1.1.1.1	Sterilised and UHT milk	E451	Triphosphates	1000.0	1000
8	NULL	A.1.1.1.1	Sterilised and UHT milk	E452	Polyphosphates	1000.0	1000
9	NULL	A.1.1.1.3	UHT goat milk	E331	Sodium citrates	4000.0	4000
10	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E425	Konjac gum and glucom	10000.0	10000.0
11	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E620	Glutamic acid	10000.0	10000.0
12	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E621	Monosodium glutamate	10000.0	10000.0
13	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E622	Monopotassium glutama	10000.0	10000
14	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E623	Calcium diglutamate	10000.0	10000
15	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E624	Monoammonium glutam	10000.0	10000
16	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E625	Magnesium diglutamate	10000.0	10000
17	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E626	Guanylic acid	500.0	500
18	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E627	Disodium guanylate	500.0	500
19	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E628	Dipotassium guanylate	500.0	500
20	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E629	Calcium guanylate	500.0	500
21	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E630	Inosinic acid	500.0	500
22	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E631	Disodium inosinate	500.0	500
23	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E632	Dipotassium inosinate	500.0	500
24	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E633	Calcium inosinate	500.0	500

Figure 54: Additive MPL Table



Figure 55: Restore Default Icon

Additives Occurrence Probabilities: Database of occurrence probabilities of for FACET food categories.

The Additives table contains information on all the different additives in FACET. Clicking on the table once will bring up a preview in the bottom right pane, showing a search box for browsing different fields. The table contains the following fields:

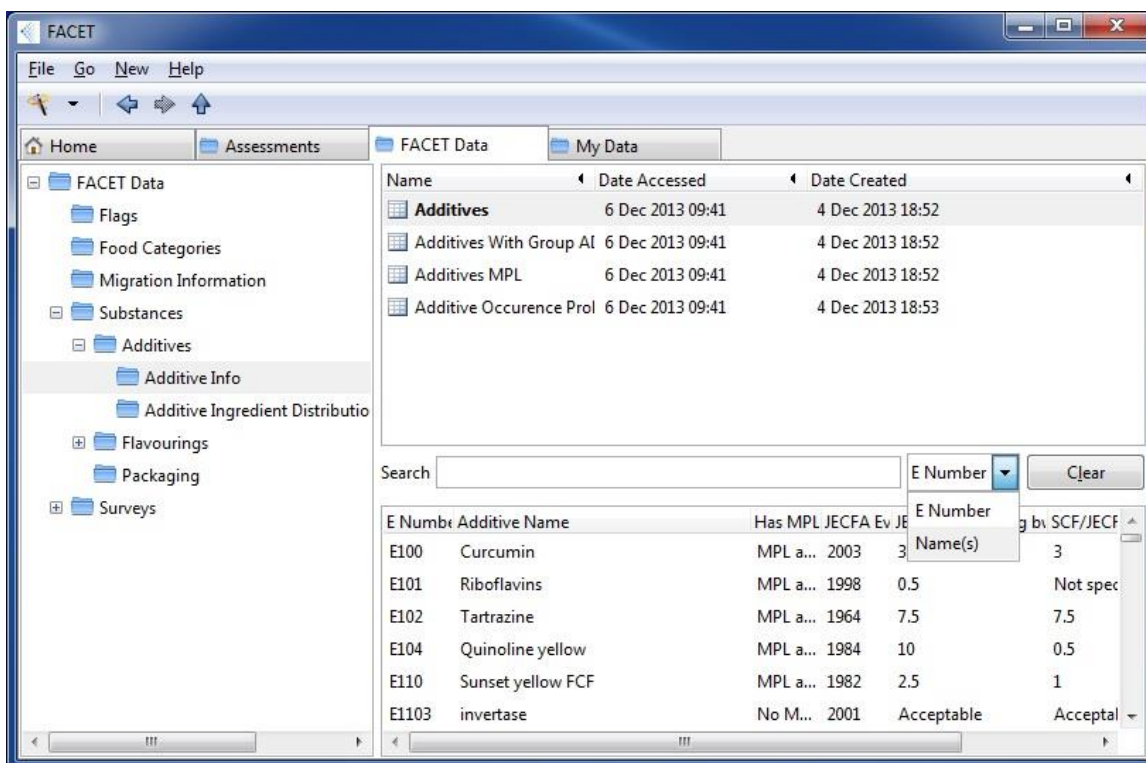


Figure 56: Additive table search box.

- **E Number:** Number given by the EU. This is the unique identifier of the additive.
- **Name:** The name(s) of the additive.
- **JECFA ADI:** Acceptable Daily Intake. This field takes a combination of numbers and letters. Units are listed in mg/kg bw, unless otherwise specified.
- **JECFA Evaluation:** Numerical field, showing the evaluation date. Entries are in a four digit year-type format (e.g. 1991).
- **SCF/EFSA ADI:** Acceptable Daily Intake. This field takes a combination of numbers and letters. Units are listed in mg/kg bw, unless otherwise specified.
- **SCF/EFSA Evaluation:** Numerical field, showing the evaluation date. Entries are in a four digit year-type format (e.g. 1991).

Additive Ingredient Distributions

This folder contains distributions of MPL concentration values for different combinations of food categories and flag settings. The distributions are used to account for the fact that an additive MPL may be set for a component of a food, e.g. in a topping. These distributions are reference in the MPL database.

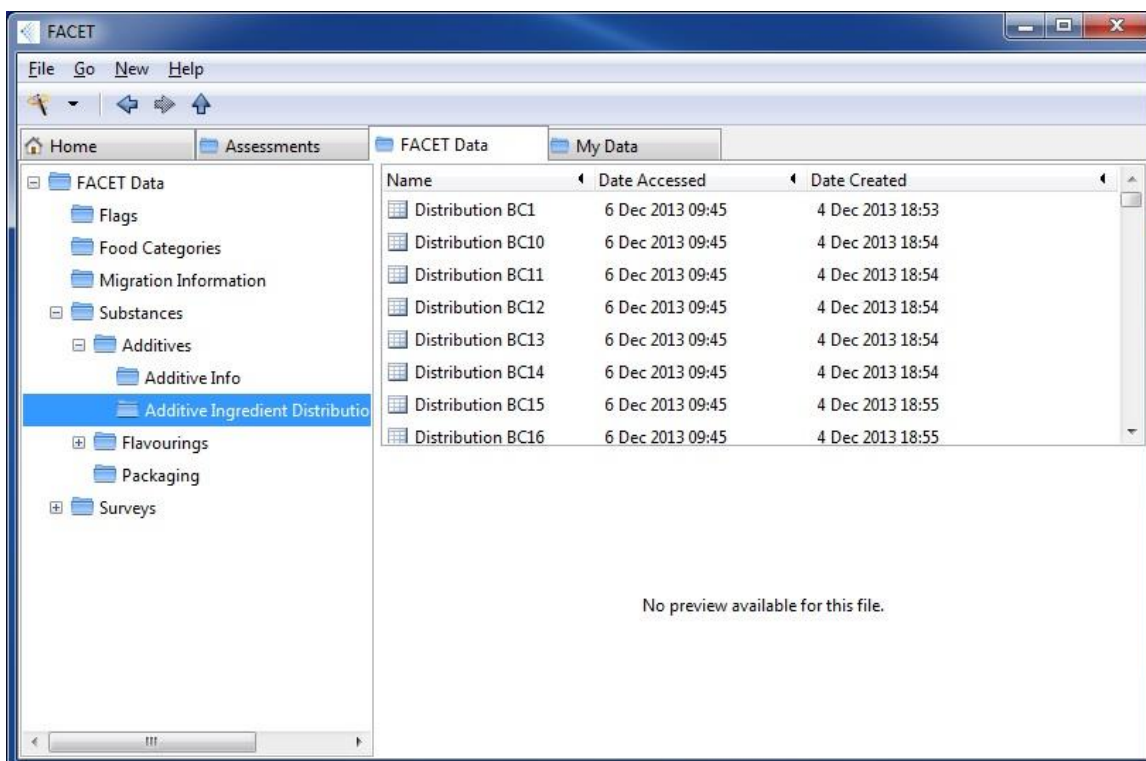


Figure 57: Additive Ingredient Distribution.

Packaging

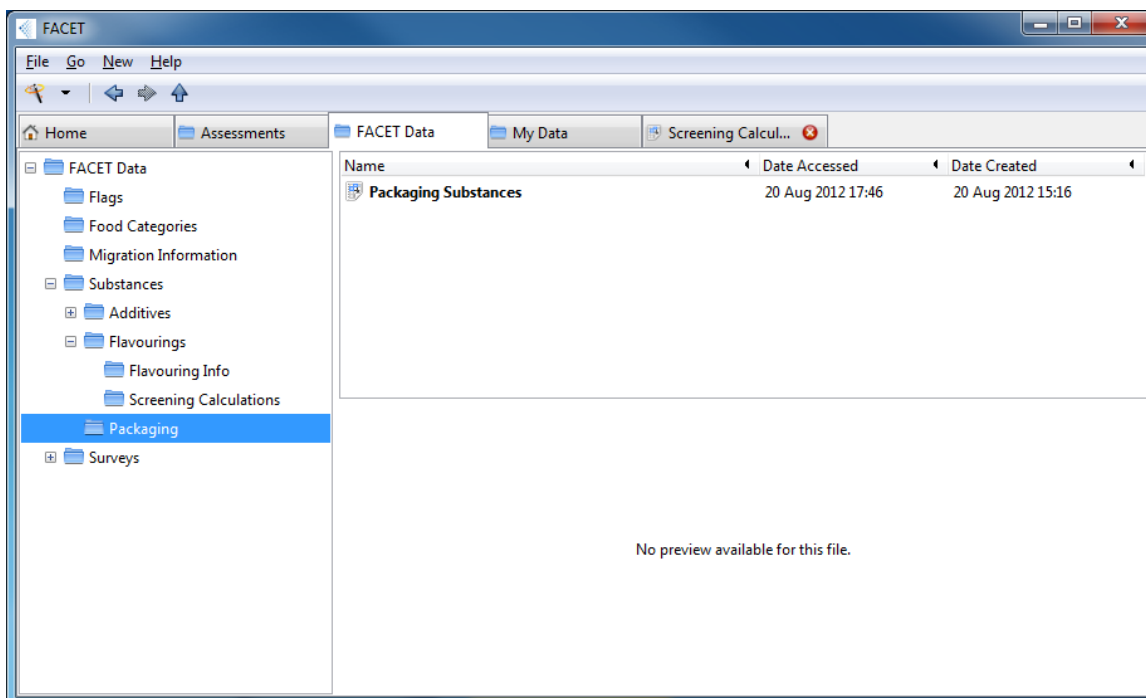


Figure 58: Packaging Folder.

The packaging folder contains one table called Packaging Substances, showing a complete list of all the packaging substances available in FACET. The table contains the following fields:

- **FACET ID:** This is strictly a four digit number with no leading zeros, e.g. “1021”. This is the unique identifier of the migrant.
- **CAS Number:** This is strictly of the form [up to 7 digits]-[2 digits]-[1 digit], e.g. “64-17-5”, or “0000064-17-5”.
- **Chemical Name:** The chemical name(s) of the substance.
- **Alternative Name:** Any other alternative names that might be associated with the substance.
- **Molecular Weight:** Molecular weight of the migrant. Strictly a numeric field.

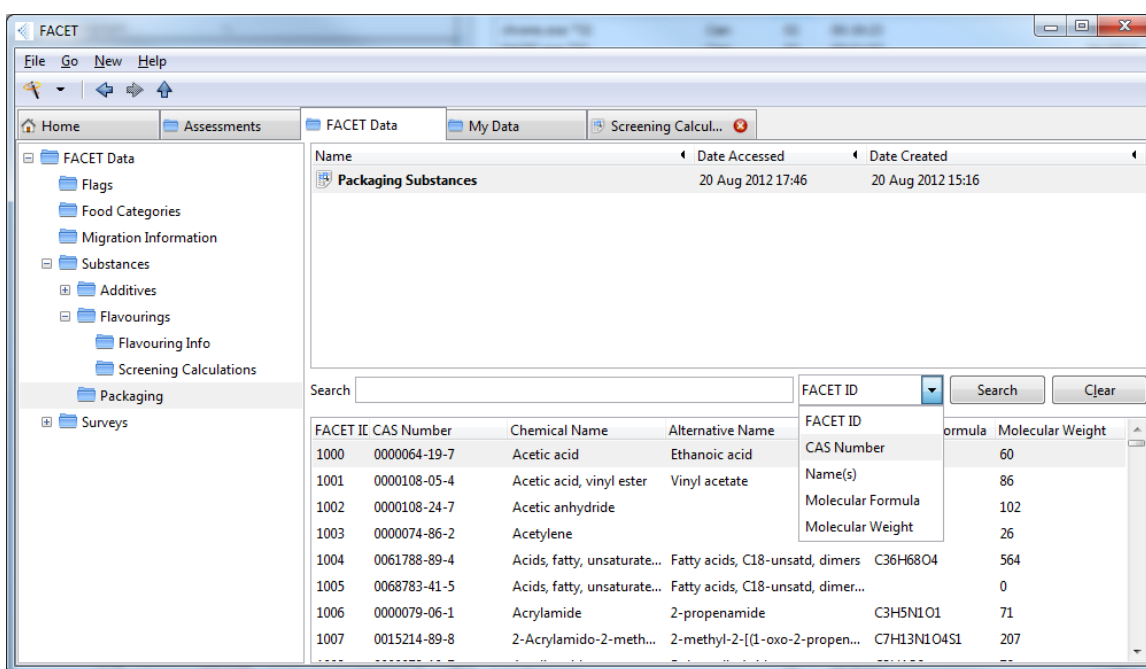


Figure 59: Packaging table search box.

Surveys

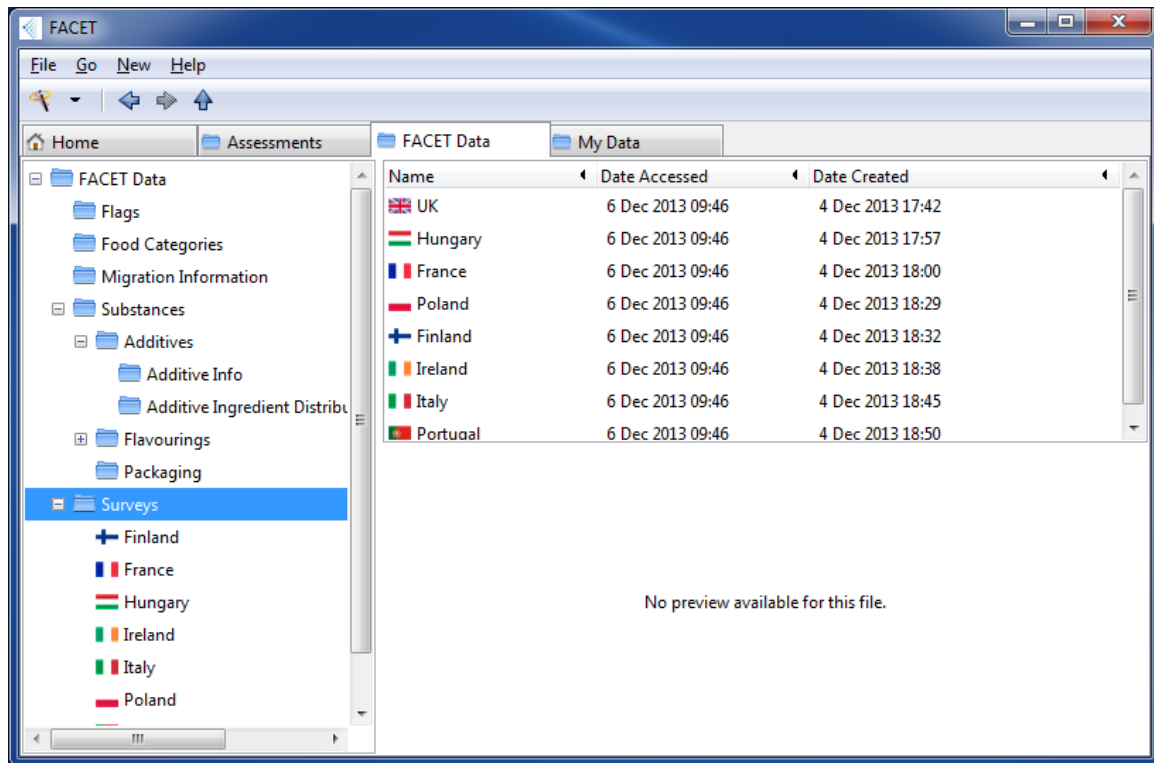


Figure 60: Surveys folder.

This allows the viewing of the various surveys available in FACET. The available surveys are the same as those that appear in Step 7 of the New Assessment Wizard. The visible fields are:

- **Name:** The name of the survey.
- **Years:** The years in which the survey was carried out.
- **Subjects:** The number of subjects in the survey.
- **Age Range:** The range of ages of subjects in the survey.
- **Methodology:** The methodology used to carry out the survey.
- **Record:** The type of dietary records that appear in the survey.

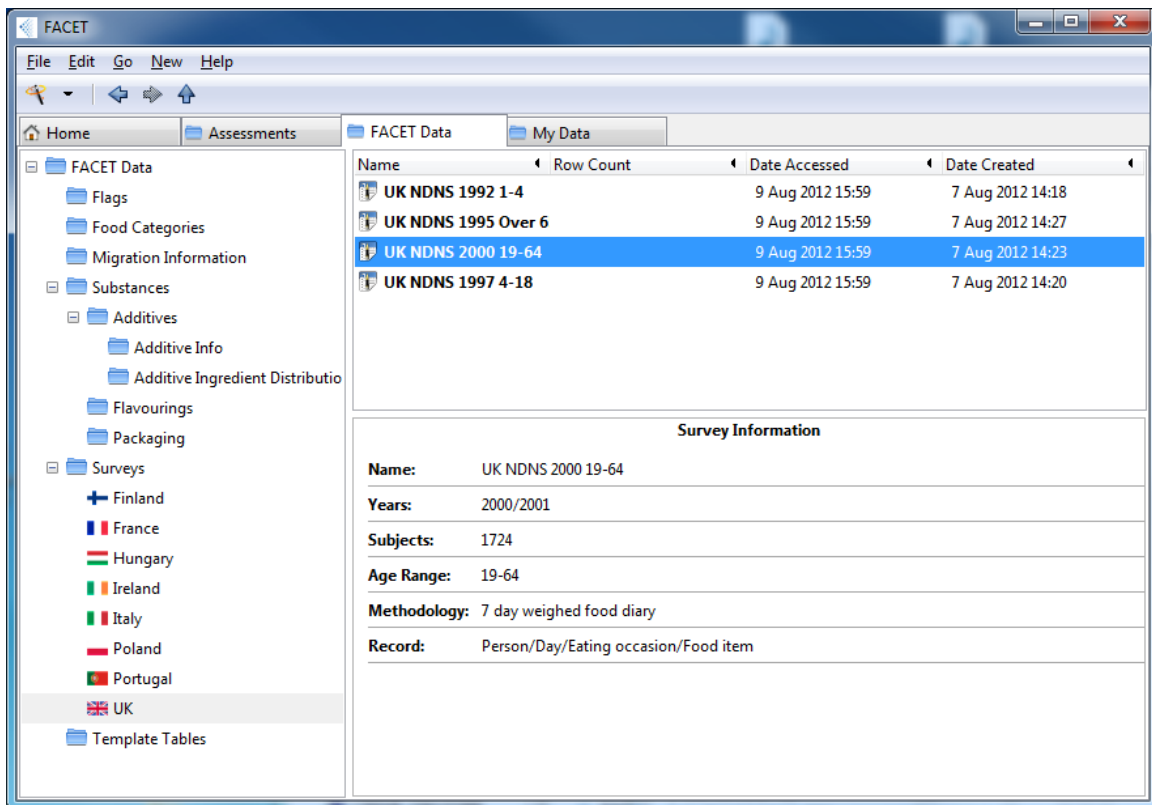


Figure 61: Visible fields in survey.

8. My Data Tab

The My Data tab is where you can create, view and edit your own data that can be used in exposure assessments. You can organise your data in a similar fashion to any file manager (e.g. Windows Explorer).

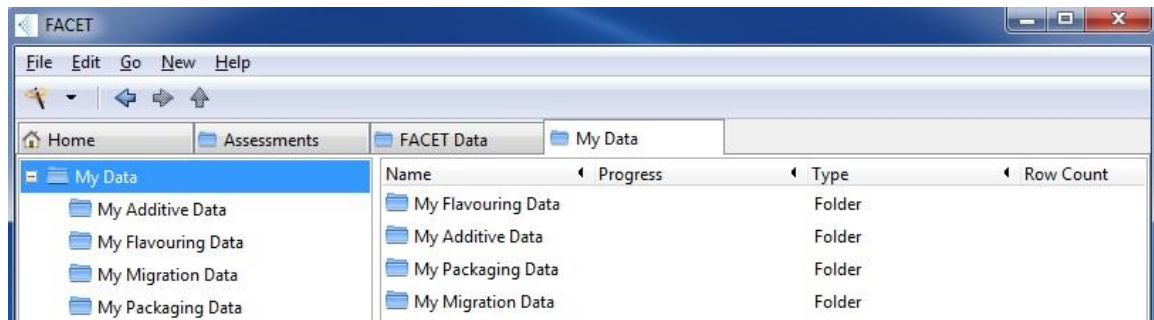


Figure 62: My Data Tab.

Managing Data

Navigating about the data manager

The My Data Tab is implemented in a two pane layout. In the left hand pane is the folder tree, which shows the hierarchy of your folders. The right-hand pane displays the contents of the current folder.

To navigate about the data manager, you can either:

1. Use the “Back”, “Forward”, and “Up” buttons in the tool bar.
2. Click on the folder whose contents you want to view in the folder tree in the left panel.

The folder structure in the left hand panel will expand or collapse to show where in the file manager you are currently viewing.

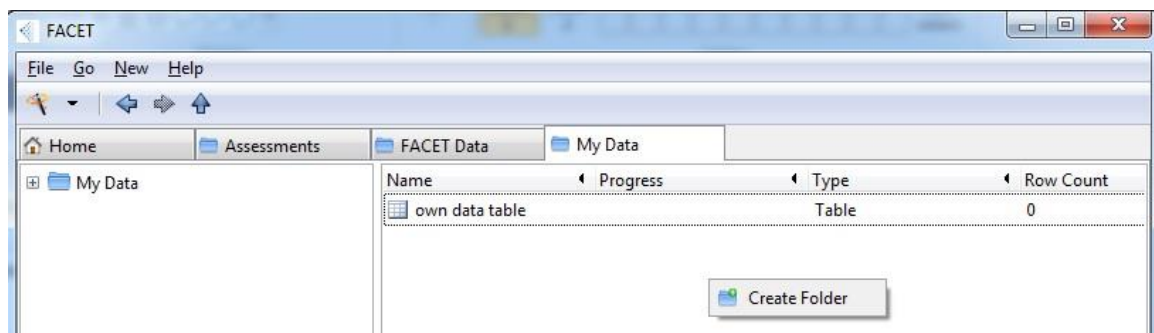


Figure 63: Example of own data table and creating new folder.

Creating a new folder

1. To create a new folder, right click on the desired location in the right pane and select “Create Folder”.
2. This will bring up a dialogue box into which one can enter the name of the new folder.
3. After entering the name of the new folder, click on “OK” and the new folder will be created.

Renaming a folder

1. To rename a folder, right click on the folder you want to rename and select “Rename”. Alternatively, select the folder and choose “Rename” from the Edit menu.
2. This will bring up a dialogue into which you can enter the new name of the folder. Enter the new name of the folder into the dialogue and click on “Rename”.

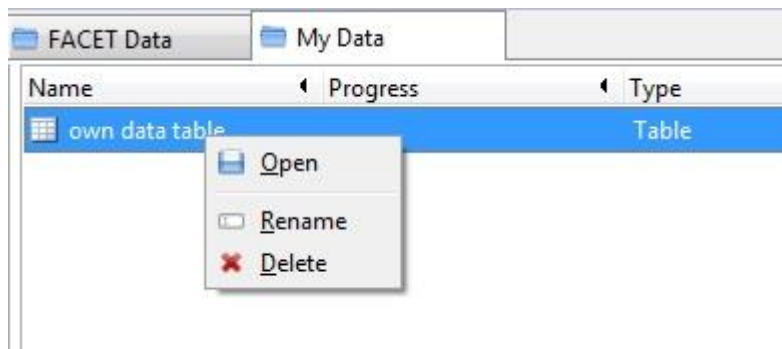


Figure 64: Renaming a folder.

Deleting a folder

1. To delete a folder, right click on the folder you want to rename and select “Delete”. Alternatively, you can select the folder and choose “Delete” from the Edit menu.

Create New Table

To create a new table in the My Data Tab for use in exposure assessments, use the Create New Table option from the “New” menu (Figure 65).

1. **Substance Type:** Select whether the table is for a new additive, flavouring, or packaging substance.
2. **Select Substance:** Select the substance that will be used for the assessment.
3. **Table Options:** Select the name and location of the table in the My Data tab by clicking on the Choose button which brings up a new name and location window.

4. **Edit the table:** The newly created table can be found in the My Data Tab in My Packaging Data. Double click on the table to open it (Figure 66).
5. **To insert a new row** into a table in the table editor, select “Insert row” from the Changes menu, or click on the “Insert row” icon (Figure 67).
6. **To delete single or multiple rows**, first highlight the required rows by clicking on the left hand margin of the relevant rows.
7. Changes to the table are saved automatically.

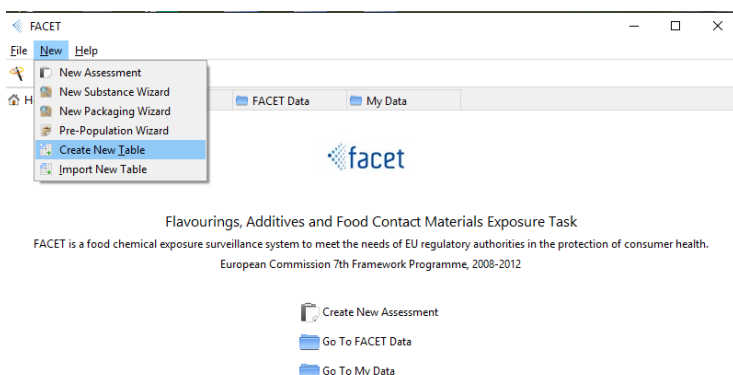


Figure 65: Create New Table

The screenshot shows the FACET application window with a new table created. The table has the following columns: FACET Description, FACET C..., Pack Type Description, Pack Type Co..., Facetid, and Chemicalna... (truncated). The table contains 15 rows of data, each with placeholder text '***'. The 'New Table' tab is active, and the table is displayed in a grid format with scrollbars.

FACET Description	FACET C...	Pack Type Description	Pack Type Co...	Facetid	Chemicalna...
***	***	***	***	***	***
***	***	***	***	***	***
***	***	***	***	***	***
***	***	***	***	***	***
***	***	***	***	***	***
***	***	***	***	***	***
***	***	***	***	***	***
***	***	***	***	***	***
***	***	***	***	***	***
***	***	***	***	***	***
***	***	***	***	***	***
***	***	***	***	***	***
***	***	***	***	***	***
***	***	***	***	***	***
***	***	***	***	***	***

Figure 66: New Table



Figure 67: Insert row using Changes menu

Entering data

User-defined concentration data requires the four types of information; concentrations, food codes, flag settings, and presence probabilities.

Concentrations

To enter a concentration value for a given row (note that the units are in mg/kg):

1. Double-click on the cell with the header "Concentration".
2. Entered the concentration data and press return. The value entered can be a number or a parametric distribution.
3. Changes to the table are saved automatically.

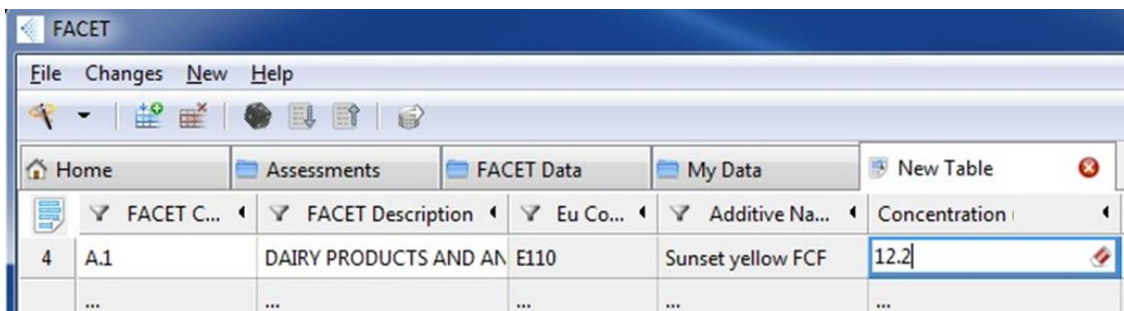


Figure 68: Entering concentration data

Presence Probabilities

To enter a presence probability for a given row (note that the value should be between 0 and 1):

1. Double-click on the cell with the header "Presence Probability".
2. Changes to the table are saved automatically.

Flag Settings

FACET flag settings can be entered by their number or description. To enter a flag setting at a given setting:

1. Double-click on the cell for the to select the desired flag, using the flag description or number, or click on the cell and press return.
2. Select from the list of available options for that cell which will appear. Double-click on the cell to enter data into it
3. Changes to the table are saved automatically.

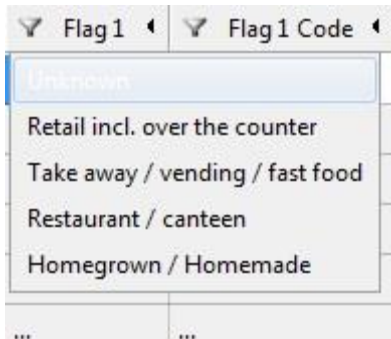


Figure 71: FACET flag settings.

9. New Packaging Wizard

There are two assessment types in the New Packaging Wizard:

1. New Pack Type
2. New Metal Pack Type

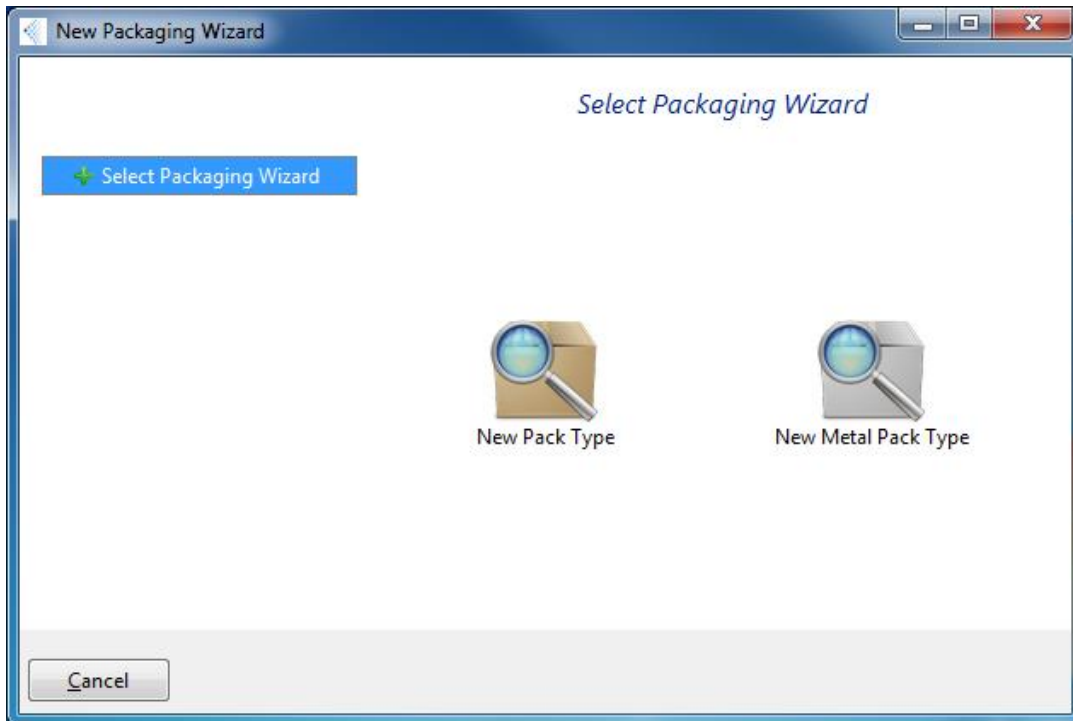


Figure 72: New packaging wizard options

New Pack Type

The New Pack Type allows users to create their own packaging materials, simulate their use in the market place in contact with specific foods and calculate the migration that is likely to ensue using a migration model. The resulting table of migration values can be viewed and used subsequently to assess the exposure to packaging additives as they are saved in the My Migration Data folder. The results can assess the impact of bringing an entirely new packaging configuration to market.

1. Select Substance

Here users can choose the substance for the assessment. This can be a newly created substance or an existing substance.

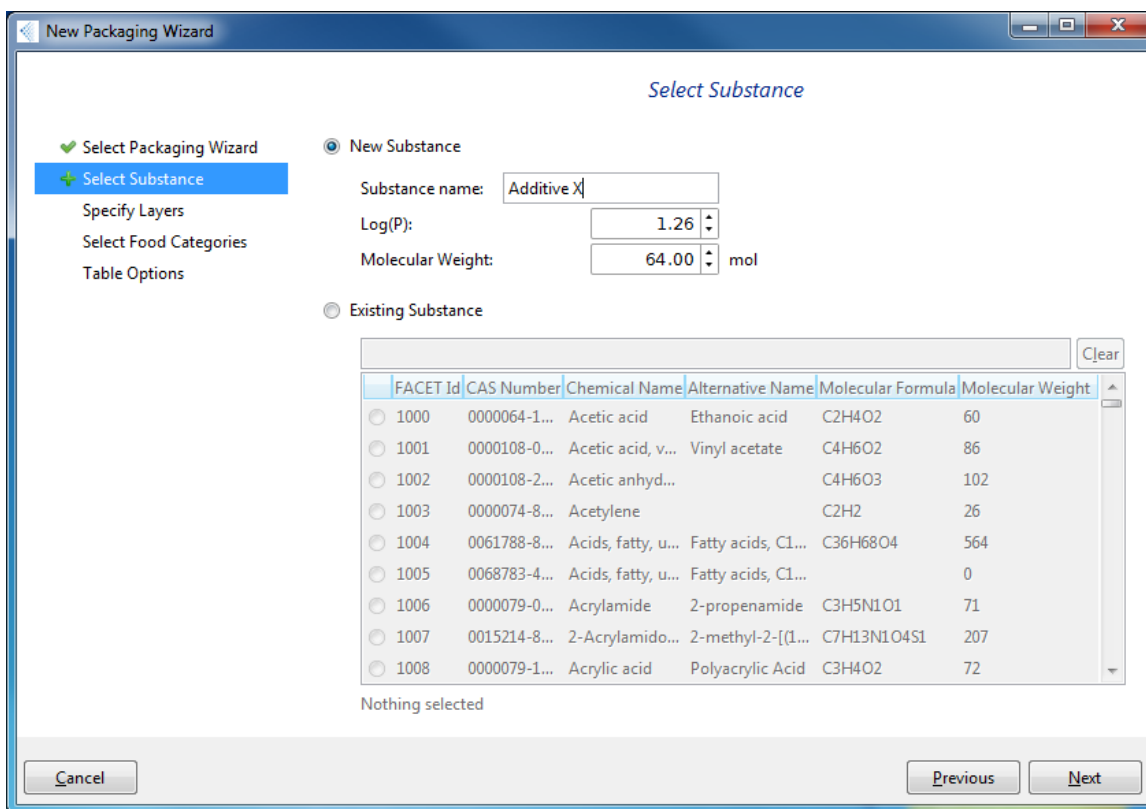


Figure 73: Create a new substance in New Packaging Wizard

New Substance

1. Enter the name of the additive in the box provided.
2. Enter the Log $P_{o/w}$ of the substance.
3. Enter the molecular weight of the substance.

Existing Substance

1. Search for the name of the substance in the search box provided.
2. Select the substance from the list.

Existing Substance

ac Clear

	FACET Code	CAS Number	Chemical Name	Alternative Name	Molecular Formula	Molecular Weight
<input type="radio"/>	1004	0061788-...	Acids, fatty...	Fatty acids, C...	C ₃₆ H ₆₈ O ₄	564
<input type="radio"/>	1005	0068783-...	Acids, fatty...	Fatty acids, C...		0
<input type="radio"/>	1006	0000079-...	Acrylamide	2-propenamide	C ₃ H ₅ N ₁ O ₁	71
<input type="radio"/>	1007	0015214-...	2-Acrylamid...	2-methyl-2-[(1...	C ₇ H ₁₃ N ₁ O ₄ S ₁	207
<input type="radio"/>	1008	0000079-...	Acrylic acid	Polyacrylic Acid	C ₃ H ₄ O ₂	72
<input type="radio"/>	1009	0002495-...	Acrylic acid,...	Benzyl acrylate	C ₁₀ H ₁₀ O ₂	162
<input type="radio"/>	1010	0000141-...	Acrylic acid,...	n-Butyl acrylat...	C ₇ H ₁₂ O ₂	128
<input type="radio"/>	1011	0002998-...	Acrylic acid,...	sec-Butyl met...	C ₇ H ₁₂ O ₂	128
<input type="radio"/>	1012	0001663-...	Acrylic acid,...	tert-Butyl acry...	C ₇ H ₁₂ O ₂	128

Nothing selected

Previous

Next

Figure 74: Search for existing substance in New Packaging Wizard

Once all of the steps have been completed, click the Submit button.

2. Specify Layers

This is where users specify the type and construction of each component of the packaging.

The layers of materials used for the construction of the packaging component can be selected from the list on the left hand side, which also has a search box at the top. The feature facilitates single layer or multi layer packaging materials and the substance of interest can be present in one or many of the layers. The order of the layers is built up from the food layer outwards.

1. At the top on the right-hand side, there are four tabs. Use these to select whether the packaging has a main, closure, outer, or insert component.
2. The user has the option to select set-off in the assessment. This is achieved by checking the "Include set-off" option.
3. The surface to volume ratio can be specified by entering the appropriate value (in dm²/kg) in the box to the right of "Surface/Volume".
4. For each tab, select the component type from the "Type" drop-down menu. If the structure doesn't have a particular component, select "Component not present" from the drop-down menu (selected by default).

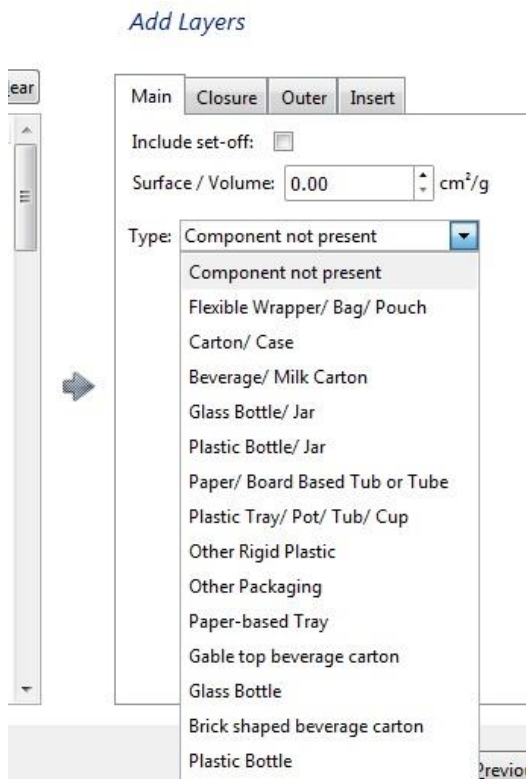


Figure 75: Select component type.

5. Add a material to the structure by selecting it from the list on the left and clicking on the blue arrow to add it to the structure (Figure 76).

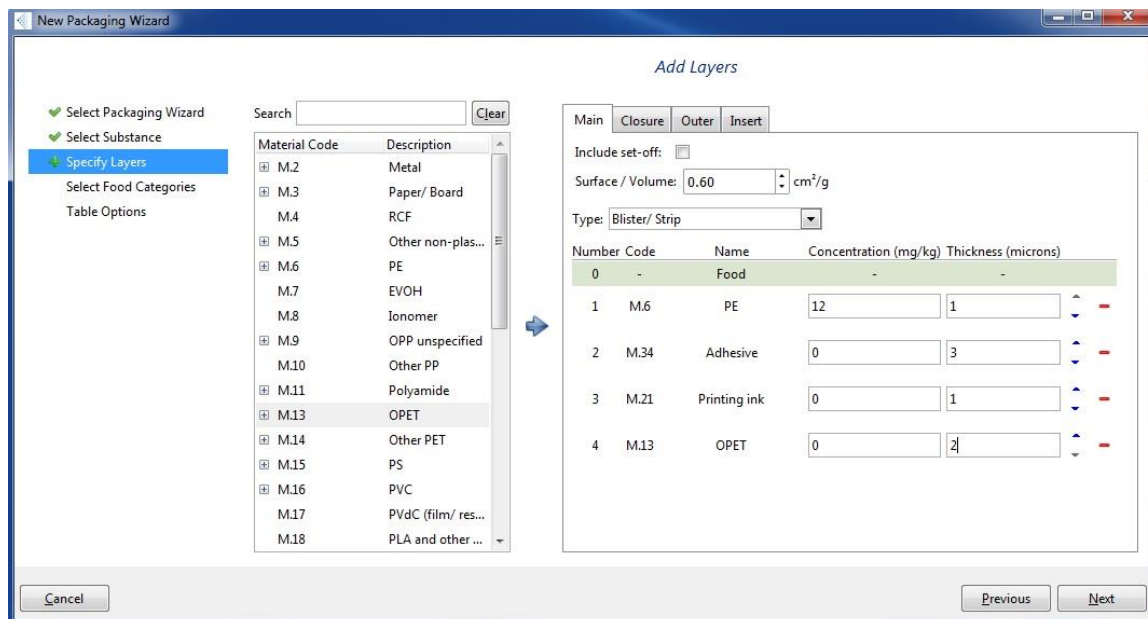


Figure 76: Add a material and specify concentration of additive and thickness of each layer

- Specify the concentration of the additive in each layer (in mg/kg) and the thickness of each layer (in microns). This value can also be a parametric distribution.
- Repeat for all required materials and components.
- The order of the layers can be re-arranged by using the black up and down arrows next to each material (Figure 76).
- Materials can also be removed by clicking on the red minus symbol next to each layer (Figure 76).

3. Select Food Categories

This is where users select the foods used for the assessment and the times and temperatures the packaging is in contact with the food. Up to five time and temperature combinations can be selected and put in order according to processing steps to create a time and temperature profile over which to calculate the migration.

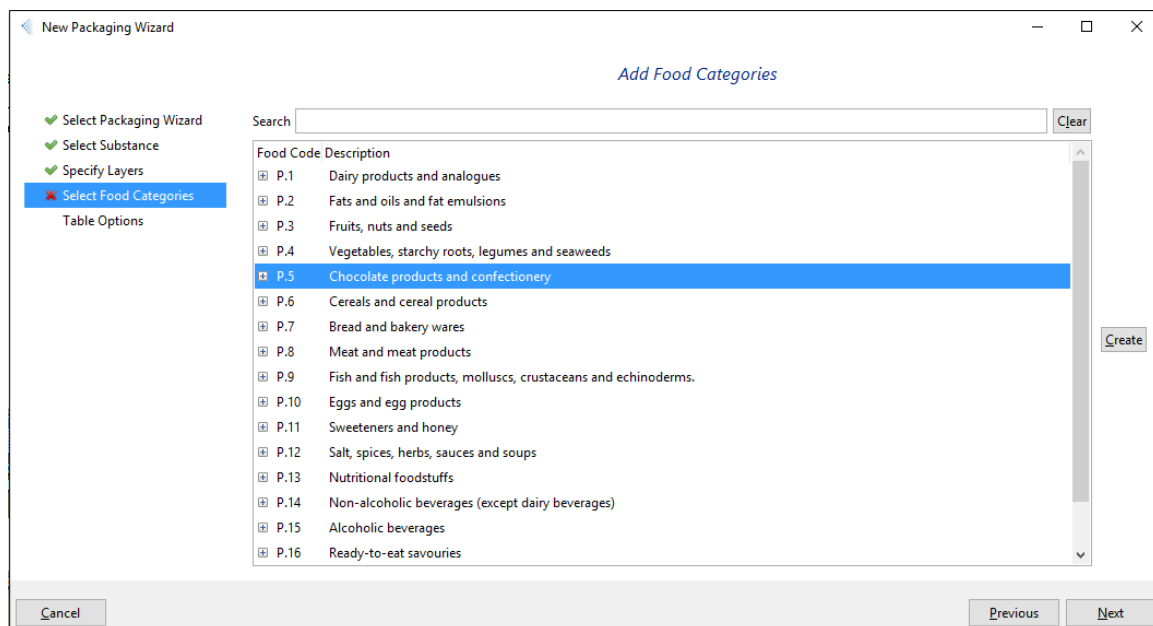


Figure 77: Select Food Category and then click Create

- The foods used for the assessment can be selected from the list, which has a search box at the top. Once a food is selected, click on the “Create” button (Figure 77). This will open a new panel on the left-hand side (Figure 78).
- At the top of the new panel, select the market share the component has in that food category by entering the appropriate value in the box.
- Enter the Pack size of the pack the new component will be used with in grams.
- In the bottom box enter the upper and lower limits of the times and temperatures the food/component combination will undergo. The units can be specified in the drop-down menus on the right-hand side.
- Additional time-temperature regimes can be added by clicking on the green plus symbol on the right-hand side.
- Time-temperature regimes can be removed by clicking on the red minus symbol on the right-hand side.

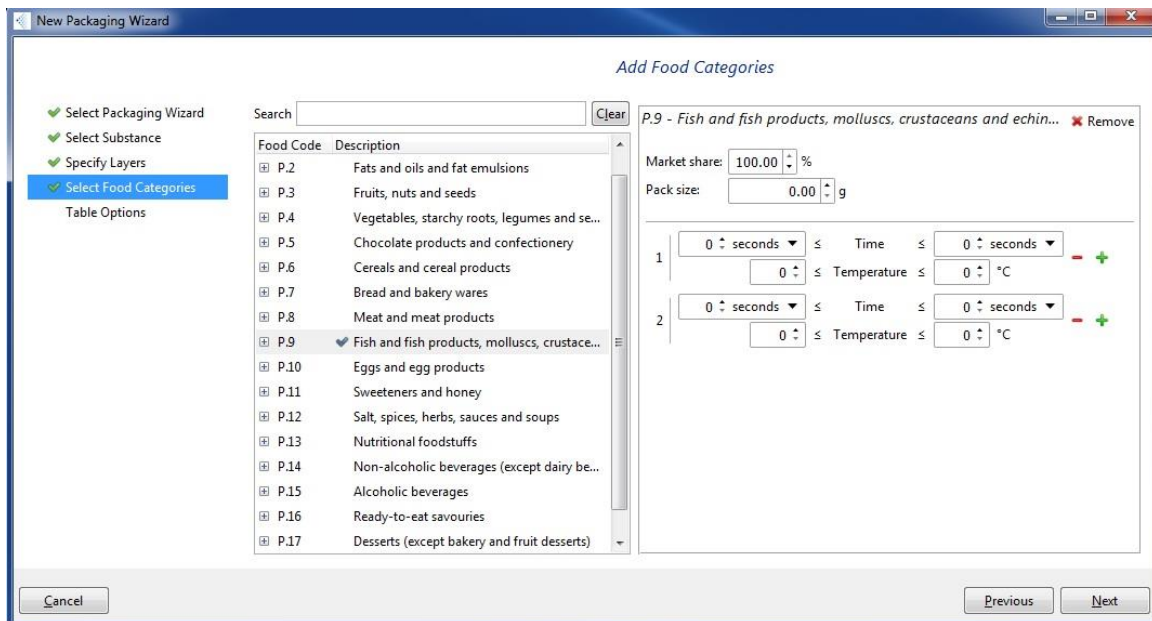


Figure 78: Insert Time Temperature profile for the selected Food Category

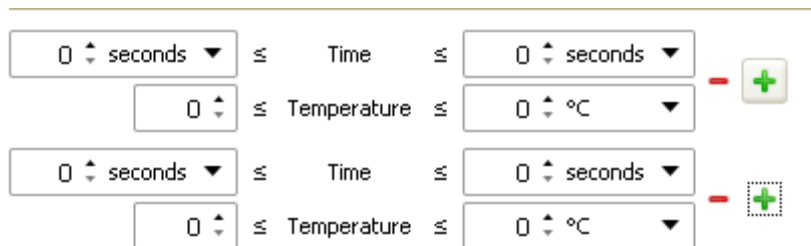


Figure 79: Additional time and temperature added using plus symbol. Remove using minus.

If desired, factory storage can also be modelled. To do this, simply click the “Include factory storage” checkbox.

4. Table Options

This step presents users with a summary of the current choices of substances, populations and food categories for the assessment.

After reviewing the choices, users can choose to start an assessment using the “Submit” button at the bottom right of the window.

Changes to the selections can be made before the assessment is submitted. To do this, navigate through the pages of the wizard by selecting them from the left of the tab.

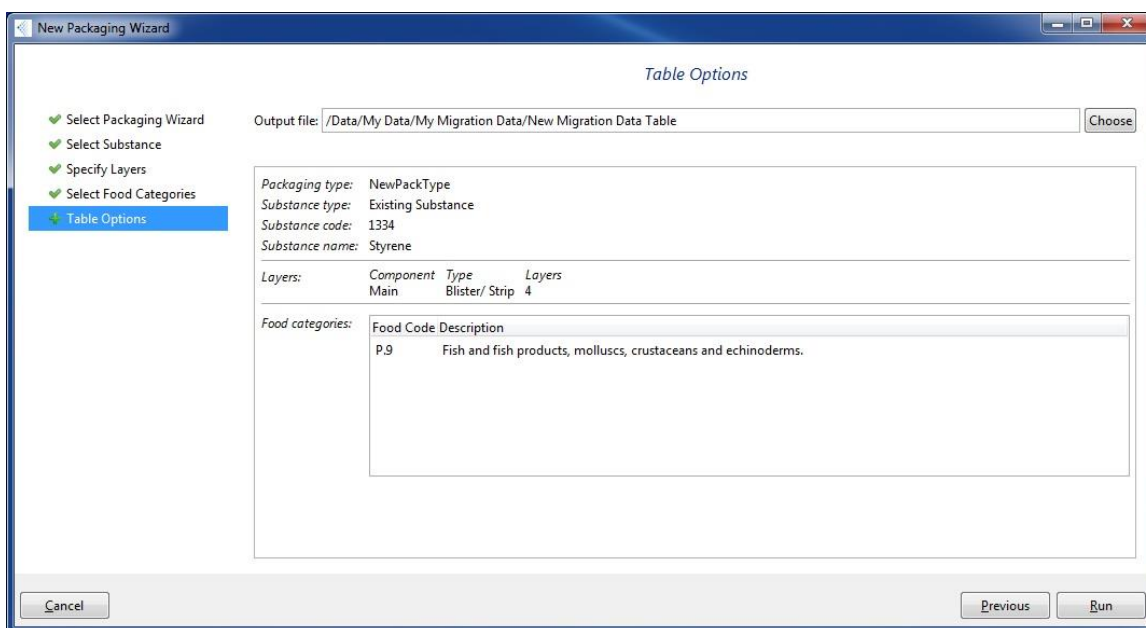


Figure 80: Table Options

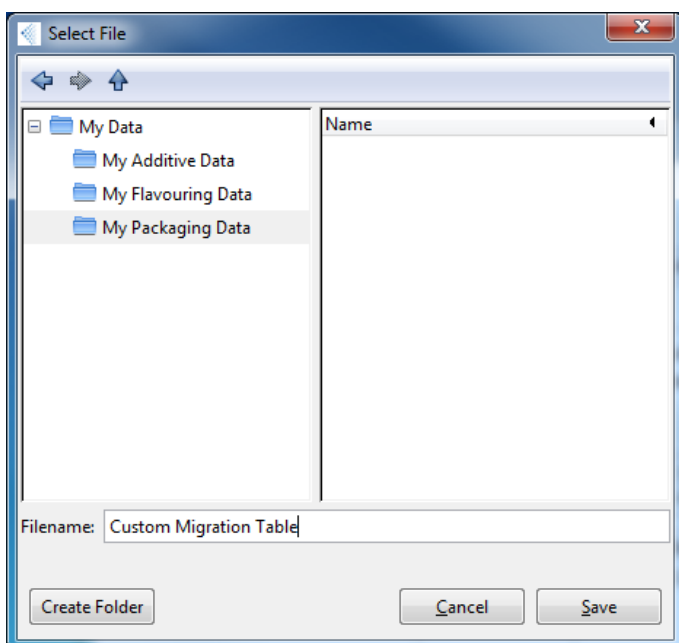


Figure 81: Saving custom migration to a file.

Limitations of the migration model

Substances with negative Log $P_{o/w}$ values when placed in a material code that is non-polar in nature will return migration values of 0 because the results for this specific combination of inputs were incalculable using the migration model.

Metal Pack Type

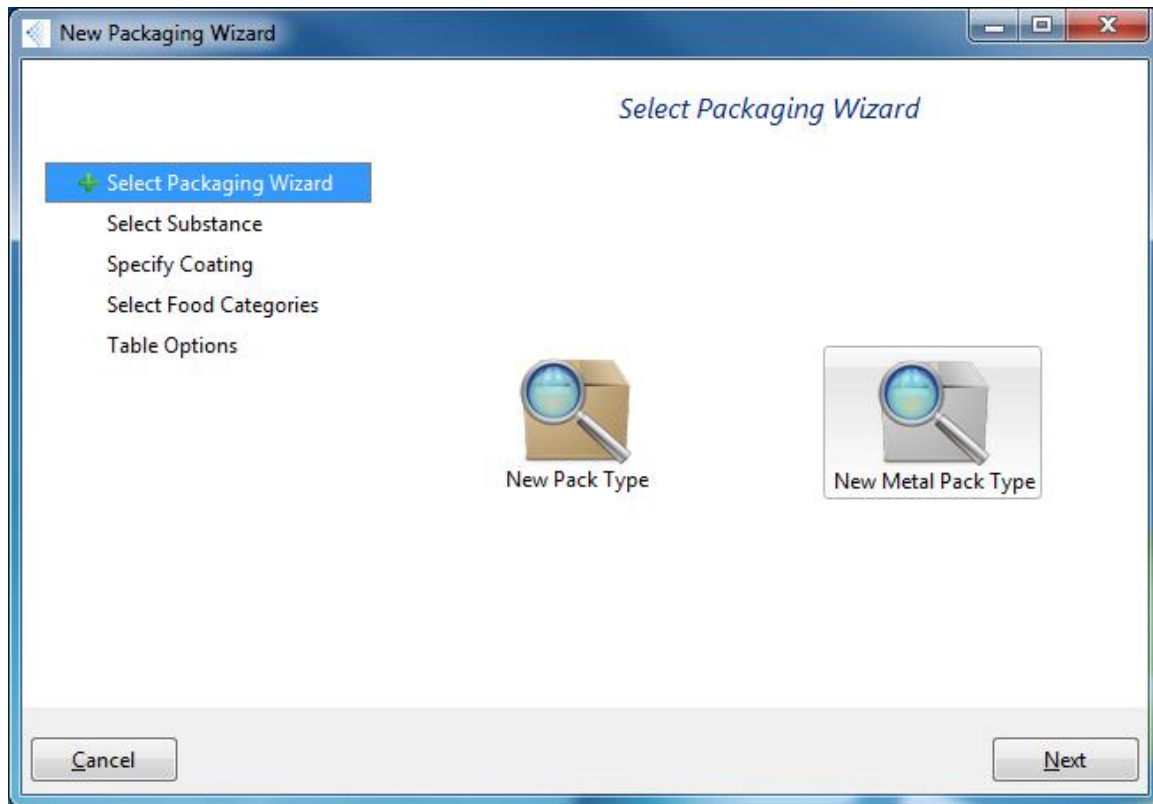


Figure 82: New metal pack type assessment.

The new metal structure feature assesses the impact of bringing an entire new metal packaging configuration to market. The migration of an additive from the components in the metal packaging into relevant foods is calculated with respect to the component use (market share) and outputted to a New Migration Table for use in an exposure assessment. This requires an additional input compared with the migration tables that are generated from non-metal New Pack Type; a migration value in mg/dm² this is because the New packaging Wizard for Metal Pack Types does not calculate migration using a migration model.

1. Select Substance

Here users can choose the substance whose level of migration to assess. It can be a new substance or an existing substance.

New Substance

1. Enter the name of the additive in the box provided and click next.

Existing Substance

ac Clear

	FACET Code	CAS Number	Chemical Name	Alternative Name	Molecular Formula	Molecular Weight
<input type="radio"/>	1004	0061788-...	Acids, fatty...	Fatty acids, C...	C36H68O4	564
<input type="radio"/>	1005	0068783-...	Acids, fatty...	Fatty acids, C...		0
<input type="radio"/>	1006	0000079-...	Acrylamide	2-propenamide	C3H5N1O1	71
<input type="radio"/>	1007	0015214-...	2-Acrylamid...	2-methyl-2-[(1...	C7H13N1O4S1	207
<input type="radio"/>	1008	0000079-...	Acrylic acid	Polyacrylic Acid	C3H4O2	72
<input type="radio"/>	1009	0002495-...	Acrylic acid,...	Benzyl acrylate	C10H10O2	162
<input type="radio"/>	1010	0000141-...	Acrylic acid,...	n-Butyl acrylat...	C7H12O2	128
<input type="radio"/>	1011	0002998-...	Acrylic acid,...	sec-Butyl met...	C7H12O2	128
<input type="radio"/>	1012	0001663-...	Acrylic acid,...	tert-Butyl acry...	C7H12O2	128

Nothing selected

Previous Next

Figure 83: Search for existing substance

New Packaging Wizard

Add Layers

- ✓ Select Packaging Wizard
- ✓ Select Substance
- ✚ Specify Coating**
- Select Food Categories
- Table Options

Search Clear

Material Code	Description
⊕ M.37	CAN COATINGS
⊕ M.38	CAN SEALANTS
⊕ M.39	METAL CLOSURE COMPO...
⊕ M.40	CLOSURE WADS

➡

Main Closure Outer

Surface / Volume: 0.00 dm²/kg

Type: Component not present

Cancel Previous Next

Figure 84: New substance in new packaging wizard metal

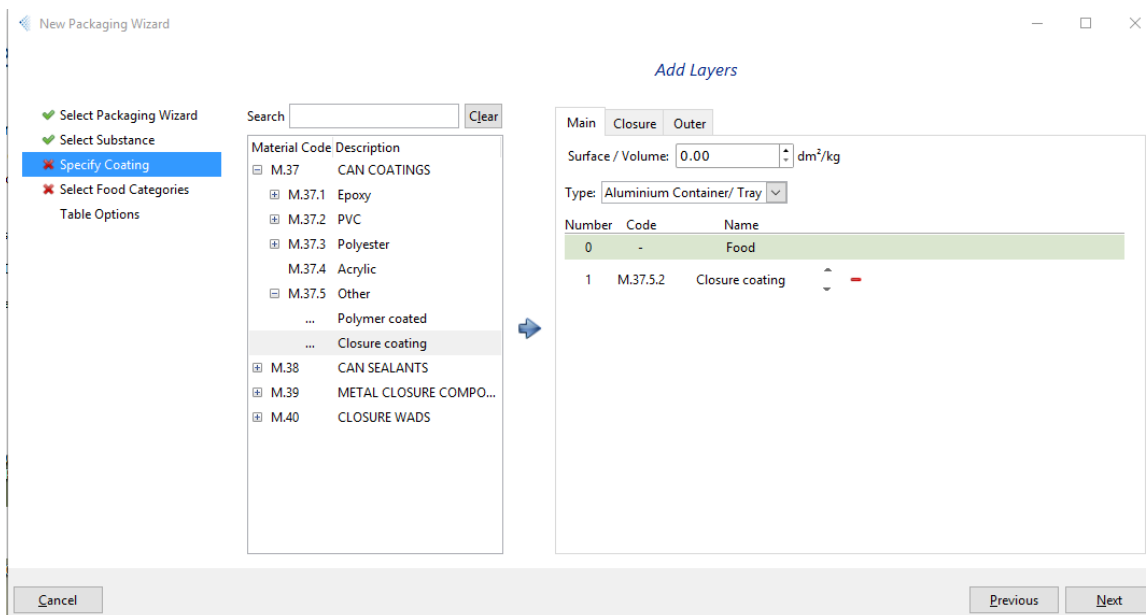


Figure 85: Selection of a metal material code

Existing Substance

1. Search for the name of the substance in the search box provided (Figure 83).
2. Select the substance from the list. Users can use the search function to speed this selection process up (**Error! Reference source not found.**).

2. Select Material

1. Enter the surface to volume ratio in Main, Closure and/or Outer (Figure 84).
2. Select what type of material this new substance is (going to be) in (Figure 85) from the metal material codes (M37 to M40).
3. Click on the blue arrow to select a material code. It will appear on the left of the window (Figure 85).

3. Select Food Categories

1. Select the foods to be used for the assessment and click on the Create Button shown in Figure 86. This will open a new panel on the left hand side (Figure 87).

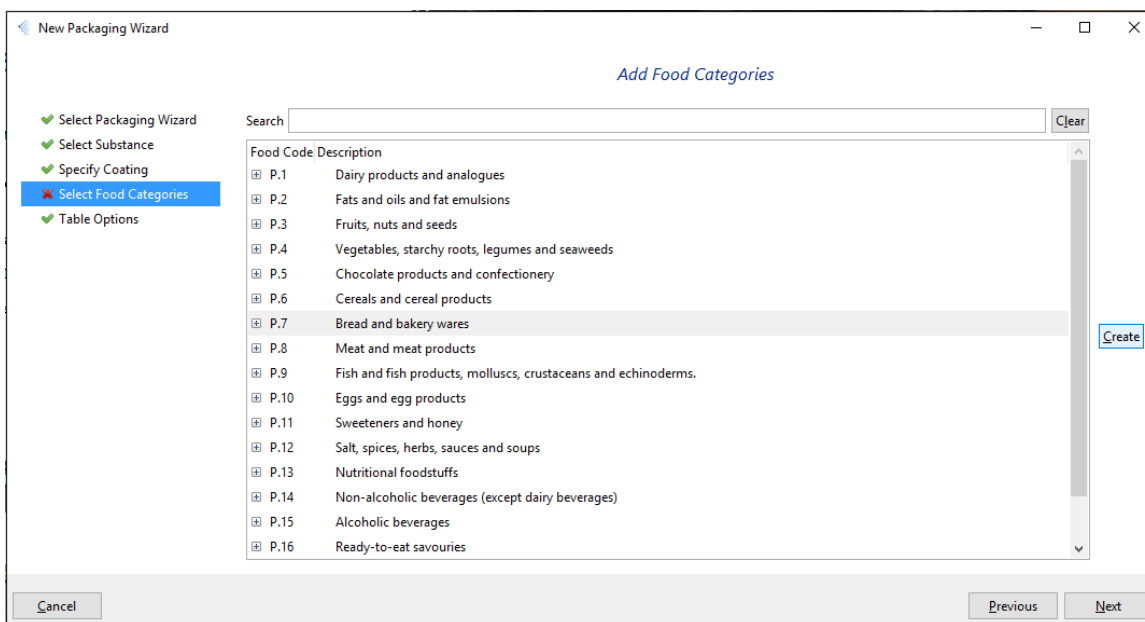


Figure 86: Select Food Category

2. At the top of the panel specific for the food category, enter a value to represent the market share the component has/ would have in the chosen food category (Figure 87).
3. Enter the weight of the pack that the new component will be/is used with (Figure 87).
4. Enter the level of migration of the substance into the food (in mg/dm^2). This value can be a single value (<1000) or a parametric distribution.
5. More than one food can be taken into consideration in the creation of a New Migration Table (The output of the New Packaging Wizard) but each food selected must get a migration profile created for it.

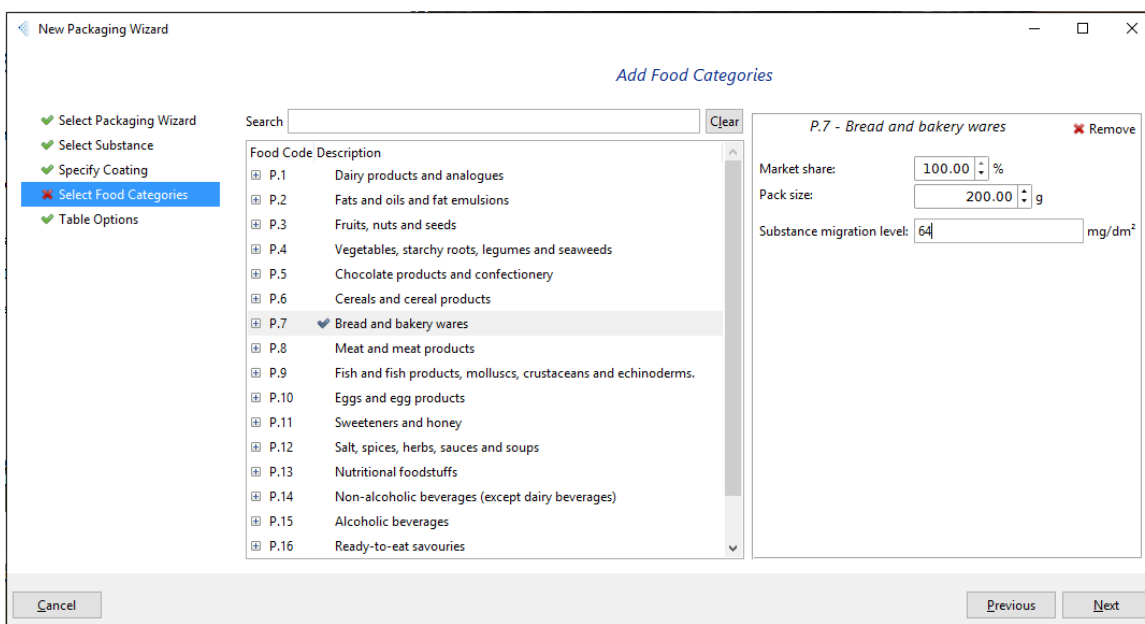


Figure 87: Create a migration profile for the selected food

4. Table Options

A summary of the selected substances, food categories, packaging details for the creation of the new Migration Data Table is shown (Figure 88).

Name the table by clicking on the Choose button. A new window will be shown where the New Migration Data Table can be named.

Changes to the selections can be made to the inputs before the table is created. To do this, navigate through the wizard table pages by selecting from them at the left hand side of the window. When all inputs have been entered, click on Run (Figure 88) to create the New Migration Data Table.

New Packaging Wizard

Table Options

✓ Select Packaging Wizard
✓ Select Substance
✓ Specify Coating
✓ Select Food Categories
✓ **Table Options**

Output file: /Data/My Data/My Migration Data/New Migration Data Table

Packaging type: NewMetalPackType
Substance type: Existing Substance
Substance code: 1334
Substance name: Styrene

Layers:	Component	Type	Layers
	Main	Aerosol can	1

Food categories:

Food Code	Description
P.8	Meat and meat products

Figure 88: Final page on the New Packaging Wizard before the creation of the New migration Data Table

10. New Substance Wizard

The New Substance Wizard can be found in the list of items available under the *New* Tab (Figure 89). It is a suite of 4 wizards where users can associate newly created substances with existing substances within packaging structures, or simply with the materials themselves used in Metal or Non-Metal packaging structures across all reported usage across all foods or a subset of foods. Users can also replace a selected existing substance up to a user specified market share. Similarly a NIAS can be created in a Non-Metal or Metal packaging structure using NIAS (Non-Metal) and NIAS (Metal) respectively, with all of the functionality of the New Substance (Non-metal) and the New Substance (Metal).

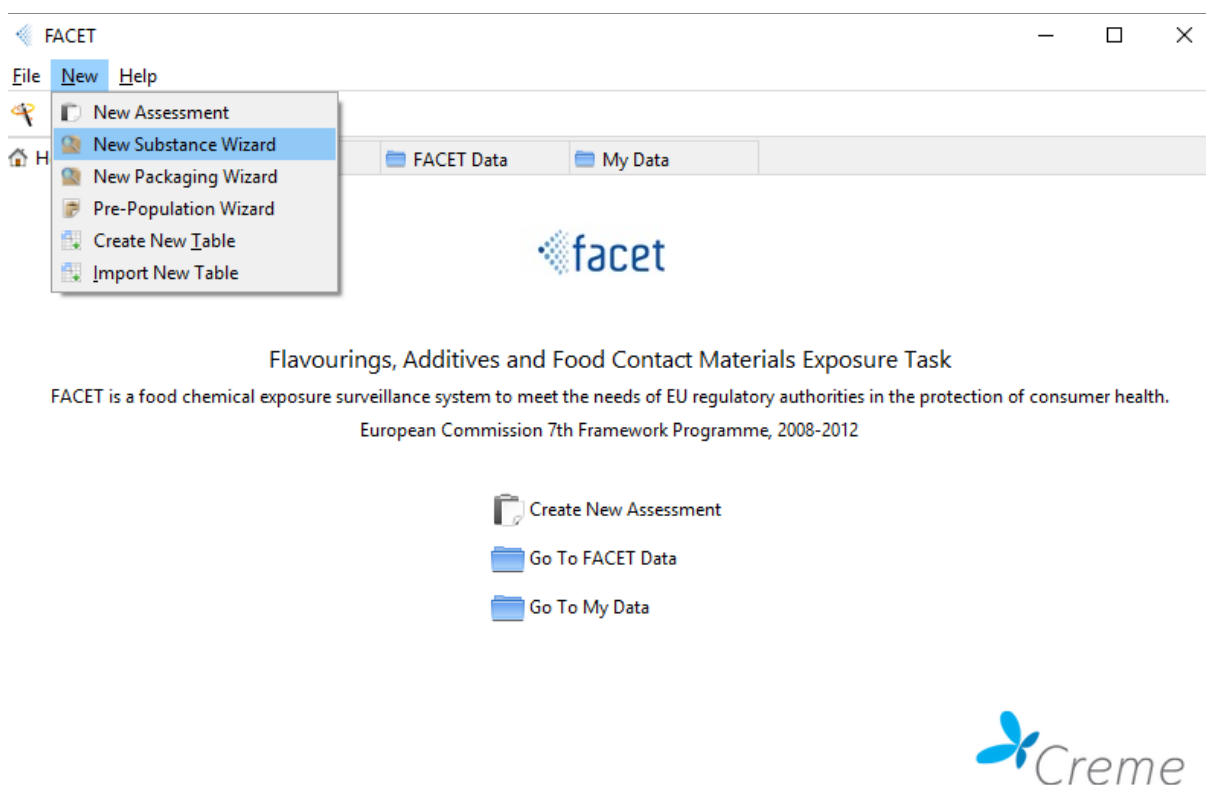


Figure 89: Location of the New Substance Wizard

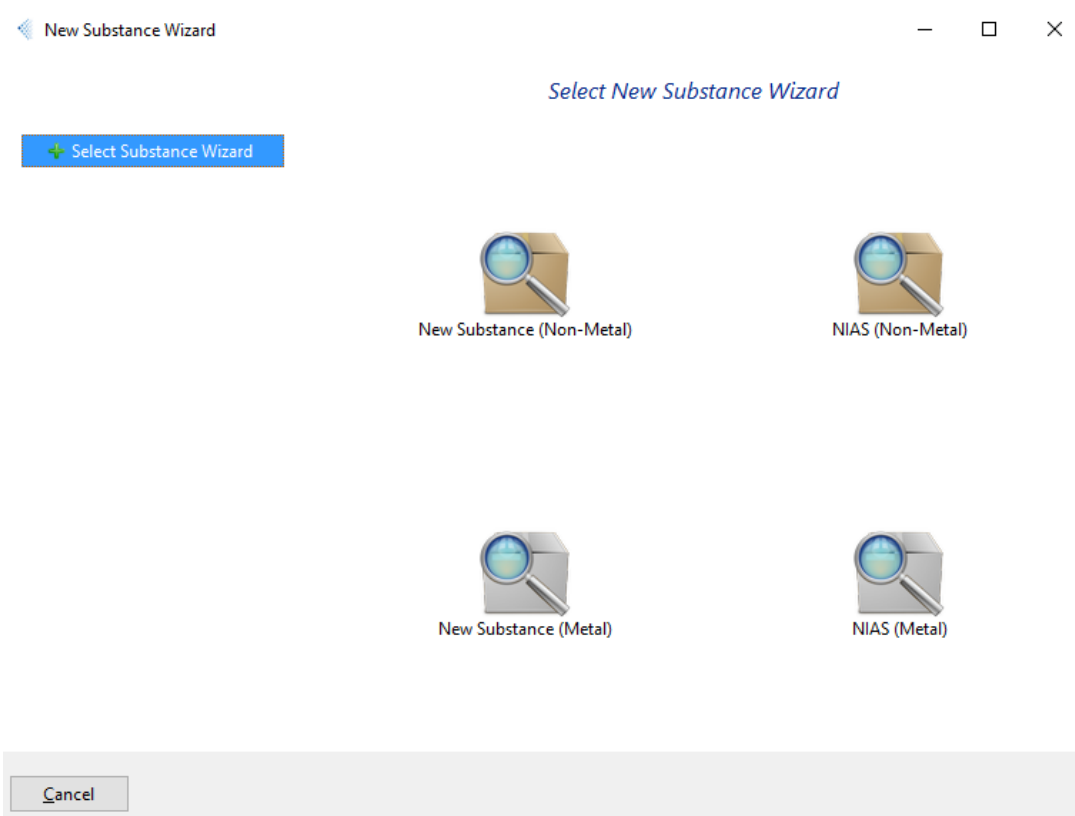


Figure 90: Four Wizard options available within the New Substance Wizard

Chose a wizard within the New Substance Wizard based on whether the substance of interest is to be associated with a Metal or Non-Metal packaging structure.

New substance (Non Metal) and NIAS (Non-Metal)

1. Name the New Substance or NIAS (Figure 91)
2. Enter the Log $P_{o/w}$ and the Molecular Weight of the New Substance or NIAS to be created.
3. Select a replacement method: Associated with an existing substance *or* Select Materials Containing Substance/NIAS

New Substance Wizard

— □ ×

Enter NIAS Details

♥ Select Substance Wizard

✦ Enter NIAS Details

Existing Substance/Materials

NIAS Concentration

Review Information

NIAS Name:

NIAS Details

Log(P):

Molecular Weight: mol

Replacement Method

☒ NIAS Associated with Existing Substance

☐ Select Materials Containing NIAS

Cancel Previous Next

Figure 91: Enter the Log Po/w and the Molecular Weight of the new substance or NIAS to be created

Replace Existing Substance/NIAS Associated with an Existing Substance

1. Select the substance to replace or associate the NIAS/Substance with (Figure 92)
2. Insert a Percentage of Existing Concentration (Figure 93). This will provide an input for the model. This is what percentage of the use of the existing substance (the one being replaced) to assign to the newly created substance or NIAS. If "50" is entered into this box, 50 % of the concentration of the existing substance in materials that its use has been reported by industry will be assigned to the new substance/NIAS.
3. Enter the Market share (Figure 93). This variable allows users to apply the above concentration (Percentage of Existing Concentration) to a percentage of the Market share of the existing substance (the one being replaced). This facilitates a more refined simulation of the introduction/existence of a newly created substance or NIAS to the market.

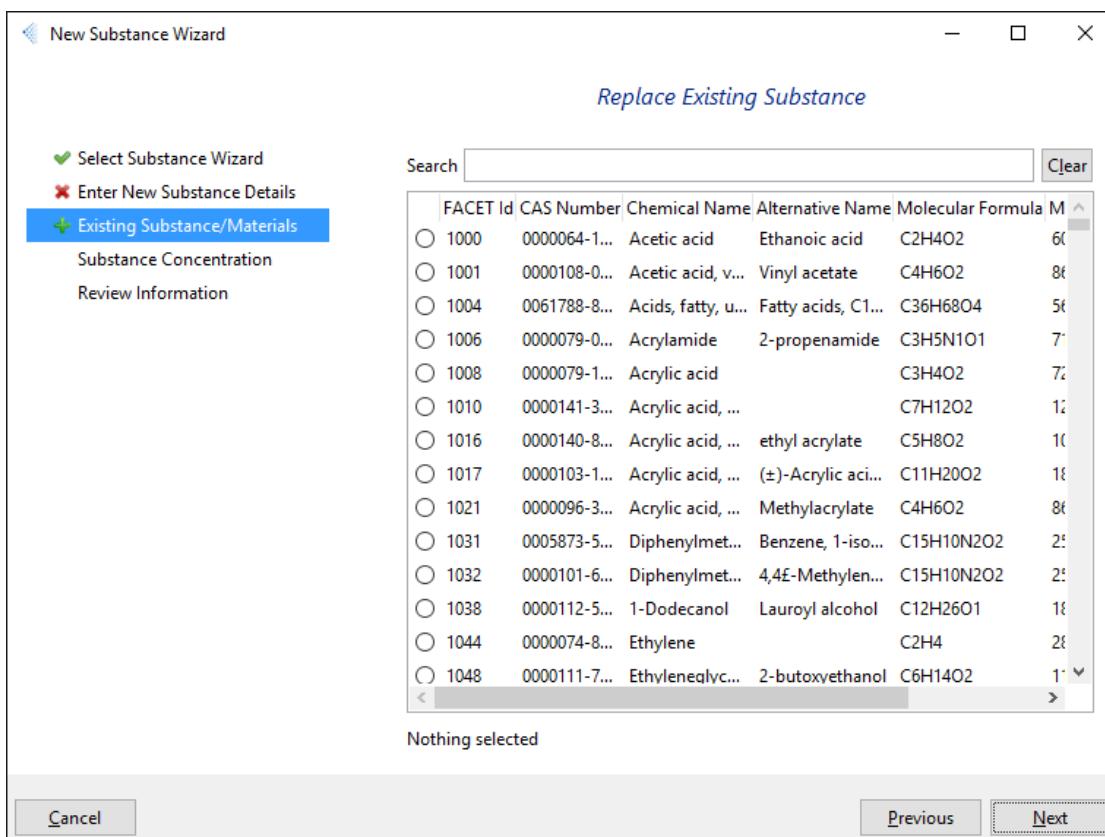


Figure 92: Select the substance to replace or associate the NIAS/Substance with

4. Select the Material Categories for which these inputs are to be simulated and click next (Figure 93)
5. A Review Information page is shown where the New Substance Wizard (Non Metal) or NIAS (Non Metal) can be named and saved. Press Run.

New Substance Wizard

Substance Concentration

- ✓ Select Substance Wizard
- ✓ Enter New Substance Details
- ✓ Existing Substance/Materials
- ✗ Substance Concentration
- Review Information

Percentage of Existing Concentration: 100.00 %

Market share: 100.00 %

Select Material Categories:

☐ Select All

Material Category

- ☐ Adhesives
- ☐ Inks
- ☐ Other coatings
- ☐ Paper and Board
- ☐ Plastics

Cancel Previous Next

Figure 93: Input page from New Packaging Wizard (non metal) or NIAS (non metal)

Select Materials Containing Substance/NIAS

1. Select, from the list of Material Codes, the materials that are to contain the new substance or NIAS (Figure 94)
2. Specify the concentration(s) of new substance or NIAS in the various material codes and the market share(s) (Figure 95)
3. A Review Information page is shown where the New Substance Wizard (Non Metal) or NIAS (Non Metal) can be named and saved. Press Run.

New Substance Wizard

Select Materials

☒ Select Substance Wizard
☒ Enter New Substance Details
☒ Existing Substance/Materials
 Enter Substance Concentrations
 Review Information

Search

☒ Select All

Code	Category Name
<input type="checkbox"/> M.1	Not Known
<input type="checkbox"/> M.2	Metal
<input type="checkbox"/> M.3	Paper/ Board
<input type="checkbox"/> M.4	RCF
<input type="checkbox"/> M.5	Other non-plastic
<input checked="" type="checkbox"/> M.6	PE
<input type="checkbox"/> M.6.1	HDPE +/- MB Additives
<input checked="" type="checkbox"/> M.6.2	LDPE +/- MB Additives
<input checked="" type="checkbox"/> M.6.2.1	LDPE without MB additives
<input type="checkbox"/> M.6.2.2	LDPE with MB additives
<input type="checkbox"/> M.6.3	VLLD or LLD +/- MB Additives
<input type="checkbox"/> M.6.4	Unspecified PE +/- MB Additives
<input type="checkbox"/> M.7	EVOH
<input type="checkbox"/> M.8	Ionomer

Figure 94: Select, from the list of Material codes, the materials that are to contain the new substance or NIAS

New Substance Wizard

Substance Concentrations

☒ Select Substance Wizard
☒ Enter New Substance Details
☒ Existing Substance/Materials
☒ Enter Substance Concentrations
 Review Information

Material Code	Concentration (ppm)	Market Share (%)
M.6		
M.6.2	7	100.00
M.6.2.1	640	6.70

Press Enter after populating the cells above

Figure 95: Specify the concentrations of new substance or NIAS in the various material codes and the market shares

New Substance (Metal) and NIAS (Metal)

The same steps as those listed for the workflow of New Substance (Non Metal) and NIAS (Non-Metal) are applicable for New Substance (Metal) and NIAS (Metal) with the exception of where users enter concentration data in the New Substance (Metal) and NIAS (Metal), in the New Substance (Metal) and NIAS (Metal) users must enter migration data (in mg/dm^2) because the New Substance (Metal) and NIAS (Metal) do not calculate migration.

The output of the New Substance Wizard

The output of running the New Substance Wizard (Non Metal), NIAS (Non Metal), New Substance (Metal) and NIAS (Metal) is the appearance of the new substance or NIAS on the list of substances available for Prepopulation in the Prepopulation Wizard. The progression of this simulation can be tracked within the *My Data* tab, in the *My Packaging Data* folder. The status of the calculation will be displayed in the *Progress* column.

11. Troubleshooting

Every effort has been made to ensure that FACET 3.0.2 is stable and error free. However, as the software is a prototype, some unforeseen issues may arise.

If the software stops working for some unknown reason, it is recommended that the following procedures be followed in sequence.

Restart the software

1. Close the software by clicking on the X in the top right corner of the main FACET window, or by selecting File and Exit. If this fails to close the program, proceed to the section called "Close FACET using the Task Manager".
2. If FACET closes successfully, restart FACET by selecting Start - > All Programs -> FACET -> FACET 3.0.2
3. If the issue is still unresolved, proceed to the section "Close FACET using the Task Manager".

Close FACET using the Task Manager

1. Press Ctrl + Alt + Delete on keyboard.
2. Click on "Start Task Manager".
3. Click on the "Processes" tab.
4. In the "Image Name" column, click on any process that begins with "FACET" to highlight it (e.g. "FACET Database.exe", "FACET Scheduler.exe", "FACET.exe", or "FACET Engine.exe"), and then click the "End Process" button.
5. Repeat this process until all of the processes whose names begin with "FACET" have been terminated.
6. Restart FACET as normal, by selecting Start - > All Programs -> FACET 3.0.2
7. If the issue is still unresolved, proceed to the section, "Reset FACET".

Uninstall and reinstall FACET

1. If all of the above fails to resolve the issue, it may be necessary to uninstall and reinstall FACET on the computer.
2. On Windows XP: Click on Start -> Settings -> Control Panel -> Add or Remove Programs
On Windows Vista: Click on Start -> Control Panel -> Programs and Features
On Windows 7: Click on Start -> Control Panel -> Uninstall a Program
In each case, see FACET 3.0.2 in the list of programs.
3. Click on FACET 3.0.2 and select "Uninstall" or "Remove". This will remove FACET 3.0.2 from your computer.
4. Create a fresh installation of FACET 3.0.2 on the computer.

12. Annex

Warnings

FACET needs to write to the hard disc and to facilitate this for Windows 8 and above it is necessary to either run as the administrator or have write permissions for the FACET folder.

Due to the age of the pre-installed FACET data and the possibility of data gaps and other inaccuracies, users are advised caution when using the pre-installed data. The recommended precaution is to compare exposure assessments and other outputs with results derived from other sources.

Run as Administrator

FACET is compatible with Windows 8 and above only when the user has administrative rights on the computer he/she is using to access FACET.

It is necessary to *run as administrator* if running on Windows 8 or above because the software needs read/write access to specific local files. To set it in his/her FACET shortcut properties:

1. Right click the desktop icon
2. Properties - Compatibility tab
3. Privilege Level - Check the 'Run as admin'
4. Apply & Ok

Data gaps

Users of the FACET tool should be aware that it has certain limitations:

- It only includes the packaging which is in direct contact with food that is sold in retail outlets and hence can only estimate the exposure to substances transferring to food out of such packaging. It does not include the transfer of substances from:
 - Secondary or tertiary packaging
 - Packaging for food supplied through the food service industries such as restaurants, take-away outlets and catering
 - Industrial packs for food supplied within the food processing industry
- The data on the occurrence and concentration of substances in packaging materials was collected from industry on a voluntary basis some years ago. Under these circumstances, it is to be expected that there might be some data gaps and inaccuracies. Users should always apply a “reality check” to their results, using exposure estimates based on different data.
- Note that such data gaps might also affect the exposure assessment of NIAS where the occurrence and concentration of the NIAS is based on the occurrence and concentration of the parent substance. Again, a reality check is recommended, e.g. by running a second assessment based on your own estimates of the NIAS occurrence and concentration in defined materials.

New Assessment/ Packaging Assessment. (Following pre-population of the substance for the selected countries)

New Assessment Wizard

Select Assessment Type ☒ Use pre-installed FACET data.

Select Migrant

Select Pack Types

Select Food Categories

Select Surveys

Assessment Options

Assessment Summary

Search

FACET IC CAS Number	Chemical Name	Alternative Name	Molecular Form	Molec. Sct	Log(P)	Sol. Ver	Pre-populated with/without	Reason not M Reported	Available For New Packaging Wizard
1567 0000112-84-5	Enucamide	cis-13-docosenoamide	C20H40N101	338	7.755	WITHOUT	TRUE	TRUE	TRUE
1605 0006680-19-8	Pentarythritol tetrakis(2-(3,5-di-tert-butyl-4-hydroxyphenyl)pr...	pentarythritol tetrakis(2-(3,5-di-tert-butyl-4-hydroxyphenyl)pr...	C73H108O12	1178	16.288	WITHOUT	TRUE	TRUE	TRUE
1617 001370-04-4	Phosphorous acid, tri(2,4-di-tert-butylphenyl)ester	tri(2,4-di-tert-butylphenyl) phosphite	C42H60O3P1	647	15.714	WITHOUT	TRUE	TRUE	TRUE
1910 0007631-86-9	Silicon dioxide	C.I. Pigment White 27	Q251	60	-0.658	WITHOUT	pigment	TRUE	TRUE
1976 000077-90-7	Tri-n-butyl acetyl citrate	Acetyltributyl citrate	C20H34O8	402	3.528	WITHOUT	TRUE	TRUE	TRUE

No substances selected.

Use my concentration data

Select Concentration Table

My Data

My Additive Data

My Flavouring Data

My Migration Data

My Packaging Data

My Pre-Population Data

Name

Date Created

Date Accessed

Use in combination with pre-installed FACET data

Cancel

Previous

Next

Warning! Due to the age of the pre-installed FACET data and the possibility of data gaps and inaccuracies, users are advised to compare exposure assessment results with results derived from other sources

New Substance Wizard/ New Substance (Non-Metal).

The screenshot shows a software window titled "New Substance Wizard" with a standard Windows title bar (minimize, maximize, close buttons). On the left is a sidebar with four steps: "Select Substance Wizard", "Enter New Substance Details" (highlighted in blue), "Existing Substance/Materials", "Substance Concentration", and "Review Information". The main area is titled "Enter New Substance Details" and contains the following fields:

- Substance Name:** A text input field.
- New Substance Details:** A section containing:
 - Log(P):** A numeric input field with the value "0.0000".
 - Molecular Weight:** A numeric input field with the value "0.01" and a unit dropdown menu currently set to "mol".
- Replacement Method:** A section with two radio button options:
 - ☒ Replace Existing Substance
 - ☐ Select Materials Containing Substance

At the bottom of the dialog are three buttons: "Cancel", "Previous", and "Next". The "Next" button is disabled. The Windows taskbar is visible at the bottom of the screen.

Warning! Selecting the “Replace Existing Substances” option makes use of the pre-loaded FACET data. Due to its age of this data and possible gaps and inaccuracies, results may be misleading and should be checked against other sources.

New Substance Wizard/ NIAS (Non-Metal).

The screenshot shows a software window titled "New Substance Wizard" with a subtitle "Enter NIAS Details". On the left is a sidebar with four steps: "Select Substance Wizard", "Enter NIAS Details" (highlighted in blue), "Existing Substance/Materials", "NIAS Concentration", and "Review Information". The main area contains the following fields:

- NIAS Name:** A text input field.
- NIAS Details:** A section containing:
 - Log(P):** A numeric input field with the value "0.0000".
 - Molecular Weight:** A numeric input field with the value "0.01" and a unit dropdown menu set to "mol".
- Replacement Method:** A section with two radio button options:
 - ☒ NIAS Associated with Existing Substance
 - ☐ Select Materials Containing NIAS

At the bottom of the window are "Cancel", "Previous", and "Next" buttons. The Windows taskbar is visible at the very bottom.

Warning! Selecting the “NIAS Associated with Existing Substances” option makes use of the pre-loaded FACET data. Due to its age of this data and possible gaps and inaccuracies, results may be misleading and should be checked against other sources.

Summary of Functionality of FACET 3.0.2

Function	What it does
New Assessment	This is for an assessment of substance exposure when a substance is in the FACET database. This means that the substance has been reported as being used by a trade association and that a mol wt and a log PoW have been assigned to the substance.
New Packaging Wizard	This can be used to assess substance migration and/or exposure for either a substance in the FACET database, or a new substance where the log Pow and mol wt are known.
New Substance Wizard, associated with an existing substance.	This is used to assess migration and/or exposure for a substance that exists at a fixed ratio (for example as a contaminant) with a substance that exists in the FACET substance database. This can be optionally restricted to specific material categories (adhesives, inks, other coatings, paper & board, plastic).
New Substance Wizard, associated with a material containing that substance.	This is used when we want to assess the migration and/or exposure of a new substance in an existing material (such as an ink). It uses the existing data within FACET for which inks are used in which applications, and what the surface to volume ratios are for these applications.
New Table Wizard.	This is used when the concentration of a migrant in the food is already known and where an assessment needs to be made of what exposure this will lead to.