



## **FACET FCM Manual**

*“Instructions and Exercises for FACET software”*

**JRC**

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# 1 Document Metadata

Document Title : FACET FCM Manual  
*Instructions and Exercises for FACET Software*

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Date : 07 October 2014

Version Number : 1.0

Client : JRC

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## **2 Objectives**

### **2.1 Introduction**

This manual sets out to provide detailed instructions to explain the functioning of the Flavourings, Additives, and food Contact materials, Exposure Task (FACET) software. This software was the end result of the 7<sup>th</sup> Framework EU funded FACET project which involved the creation of a food chemical exposure surveillance system, which covers representative regions of the EU, to meet the needs of the EU regulatory authorities in the protection of consumer health.

The manual provides step by step instructions, using screenshots from the software, for each of the assessment types available in FACET. The manual also serves to highlight the capabilities of FACET

### **2.2 Outline Structure of this Manual**

Each subsection of Section 3 considers a particular Assessment Type and provides instructions, aided by screenshots from the software, to complete the assessment. Also, each subsection finishes with exercises appropriate to the content of that subsection.

### 3 Programme Details

This section provides instructions, using screenshots from the FACET software, to aid the user in the execution of the various assessment types available in FACET.

#### 3.1 Running a Basic Packaging Assessment

To run a basic packaging assessment requires the user to initially select the “Create New Assessment” option. This is described in Figure 3-1 below.

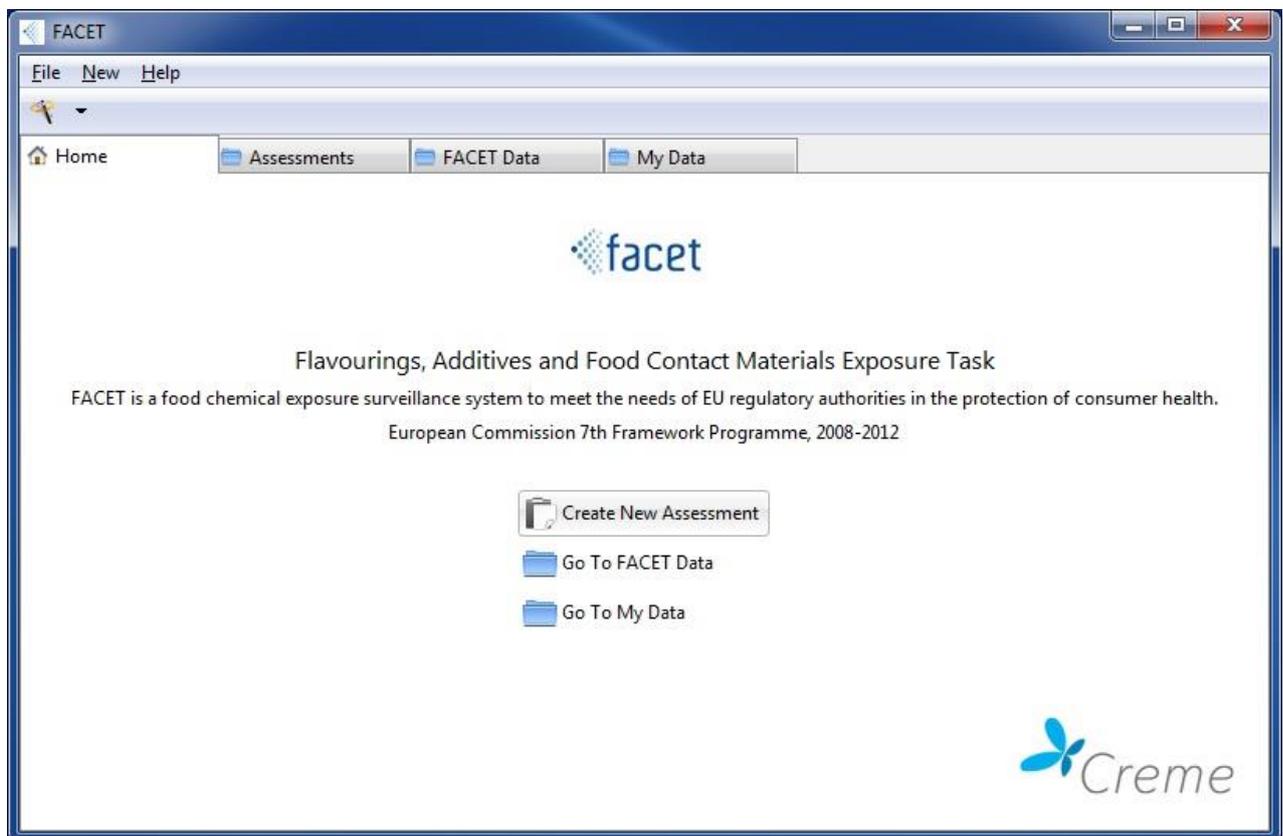


Figure 3-1: Create New Assessment

The user now has the option to select the particular assessment type they are interested in. In our case, we would like to run a Packaging Assessment and for this reason, we select the “Packaging Assessment” option, as shown in Figure 3-2 below.

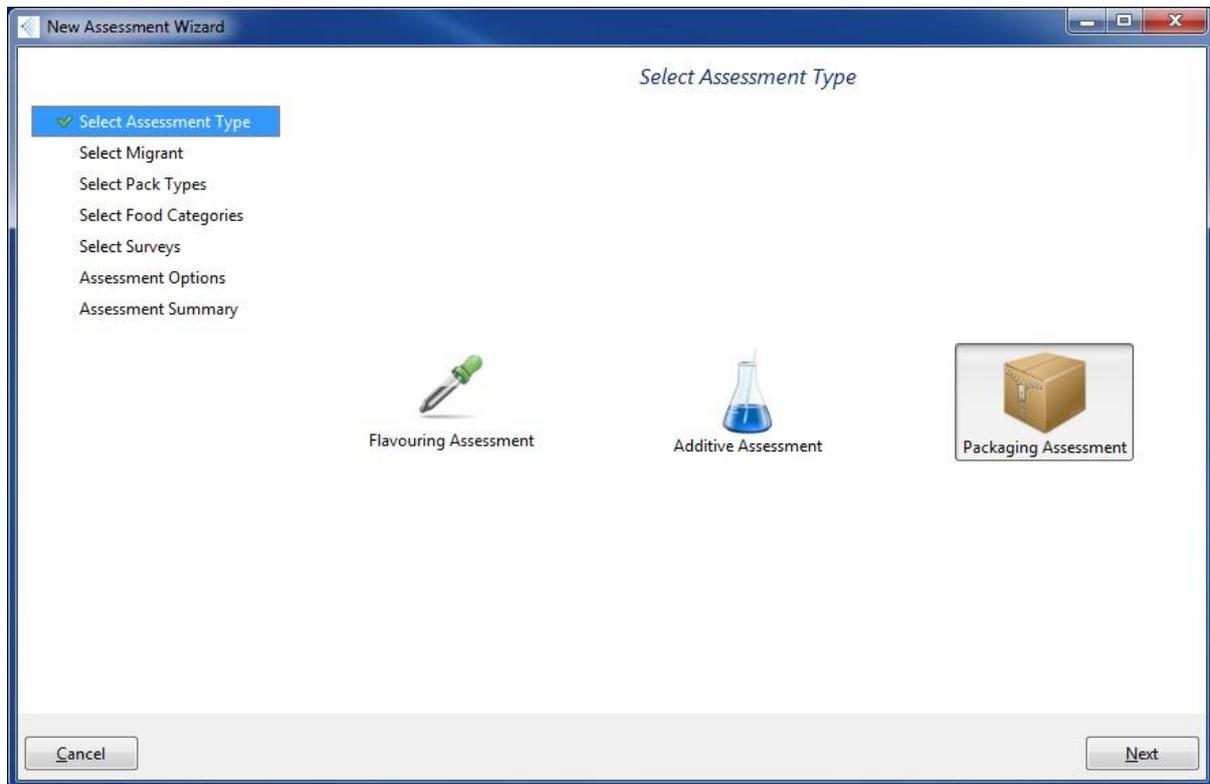


Figure 3-2: Selection of Assessment Type

Once the user selects the “Packaging Assessment” type, and clicked the “Next” button”, the next step requires them to select a migrant/substance the user would like to calculate an exposure to from different foods and pack types.

There are two options at this stage – the first option allows the user to avail of pre-installed concentration data for the substance while the second option allows the user to enter their own concentration data. For this run, we choose the “Use pre-installed FACET data” option and then select the substance BPA (FACET ID = 1084) as shown in Figure 3-3.

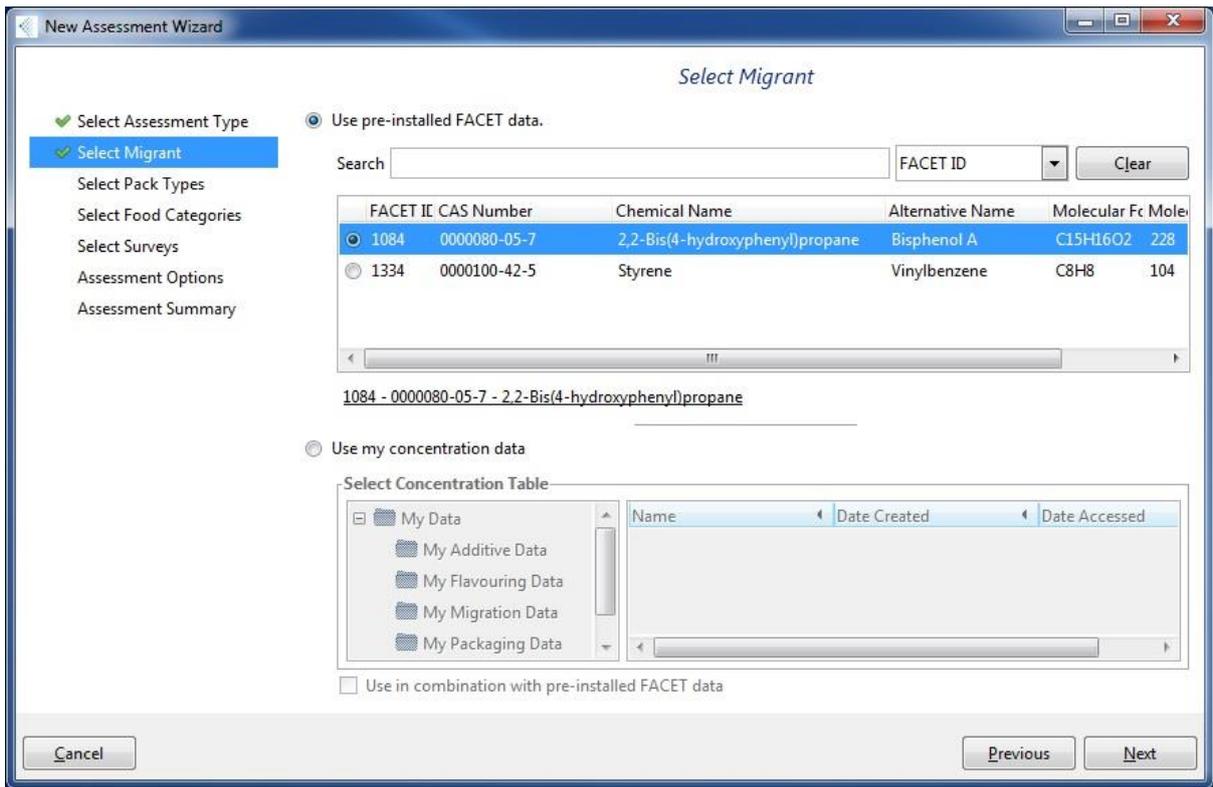


Figure 3-3: Selection of Substance

Once the substance is selected, and the “Next” button” is clicked, the user selects the “Pack Types” of interest. This step is described in Figure 3-4.

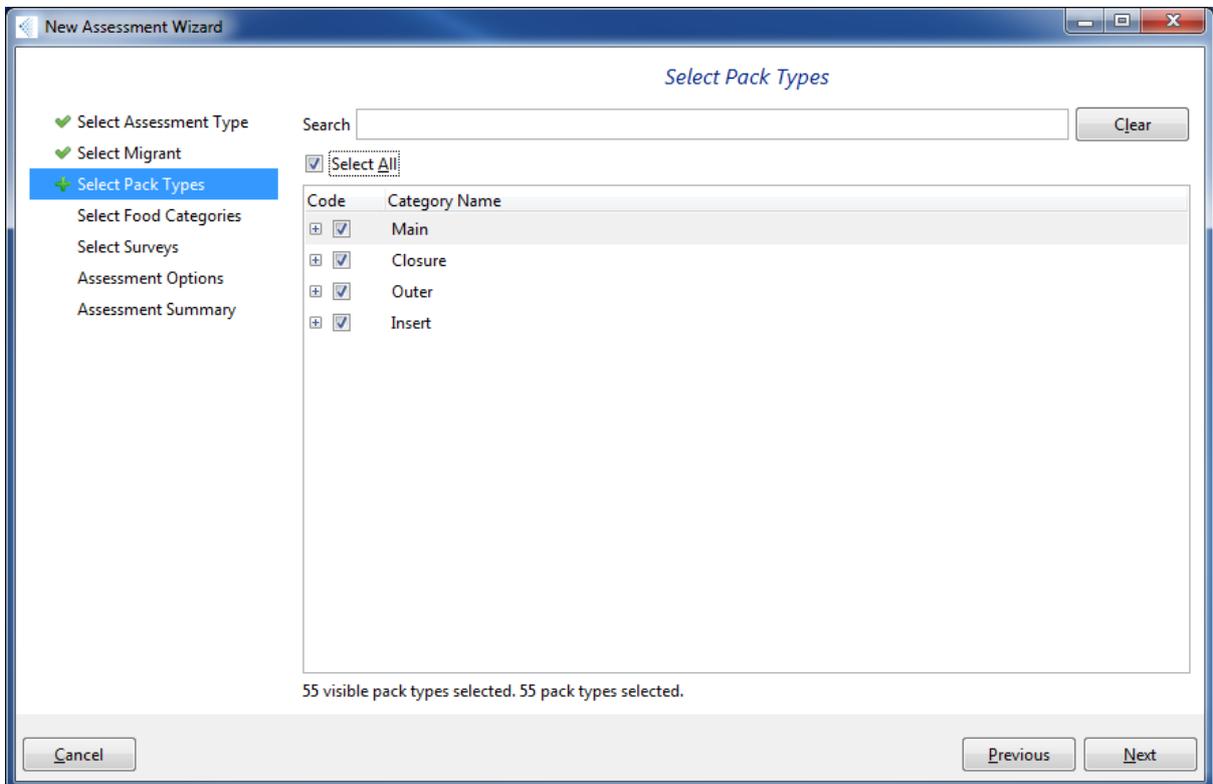


Figure 3-4: Selection of Pack Types

As well as the selection of pack types, the user also has the option to choose particular foods for the exposure assessment. This is illustrated in Figure 3-5. As with the previous steps it is required to click the “Next” button to advance to the next step.

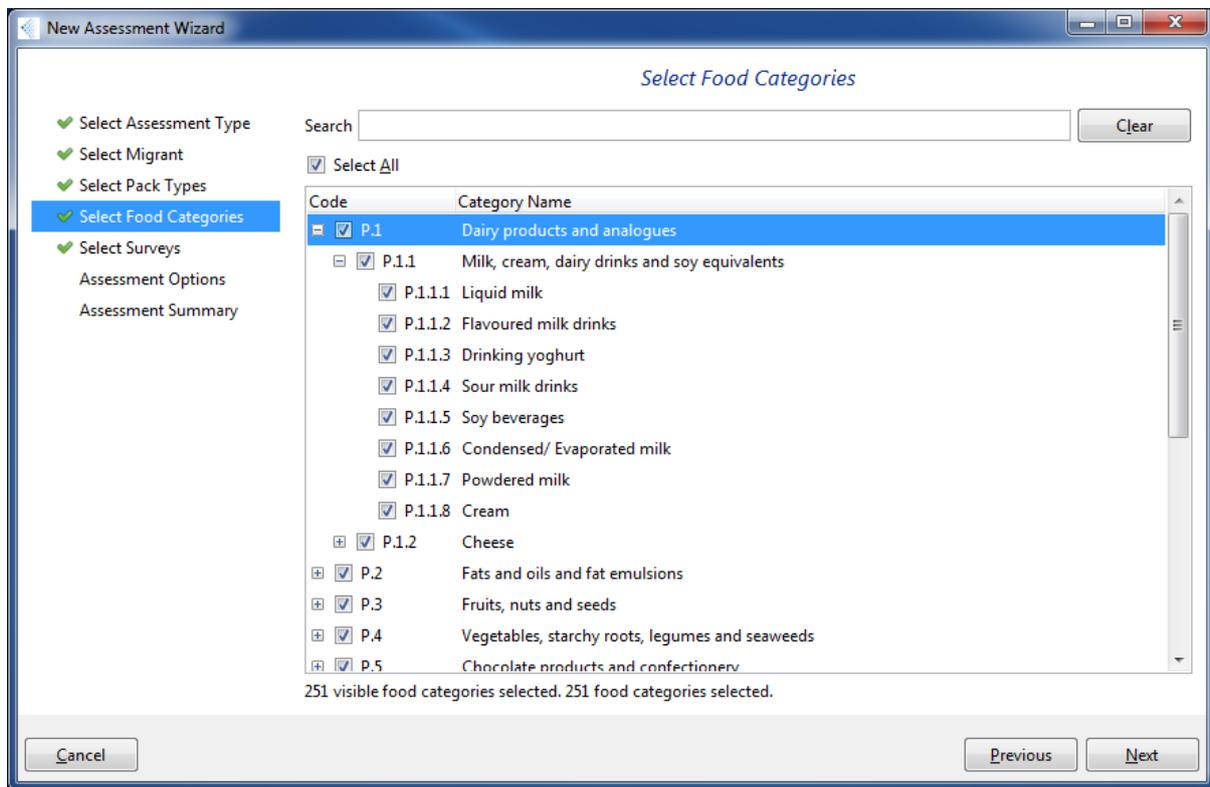


Figure 3-5: Selection of Foods

There are fifteen consumer surveys available to use in FACET. By selecting a particular survey, the software returns the exposure to the chosen substance for the population represented in the survey. In this case we select the “UK NDNS 2000 19-64” survey, as shown in Figure 3-6. This survey concentrates on people in the age group 19-64 in the UK.

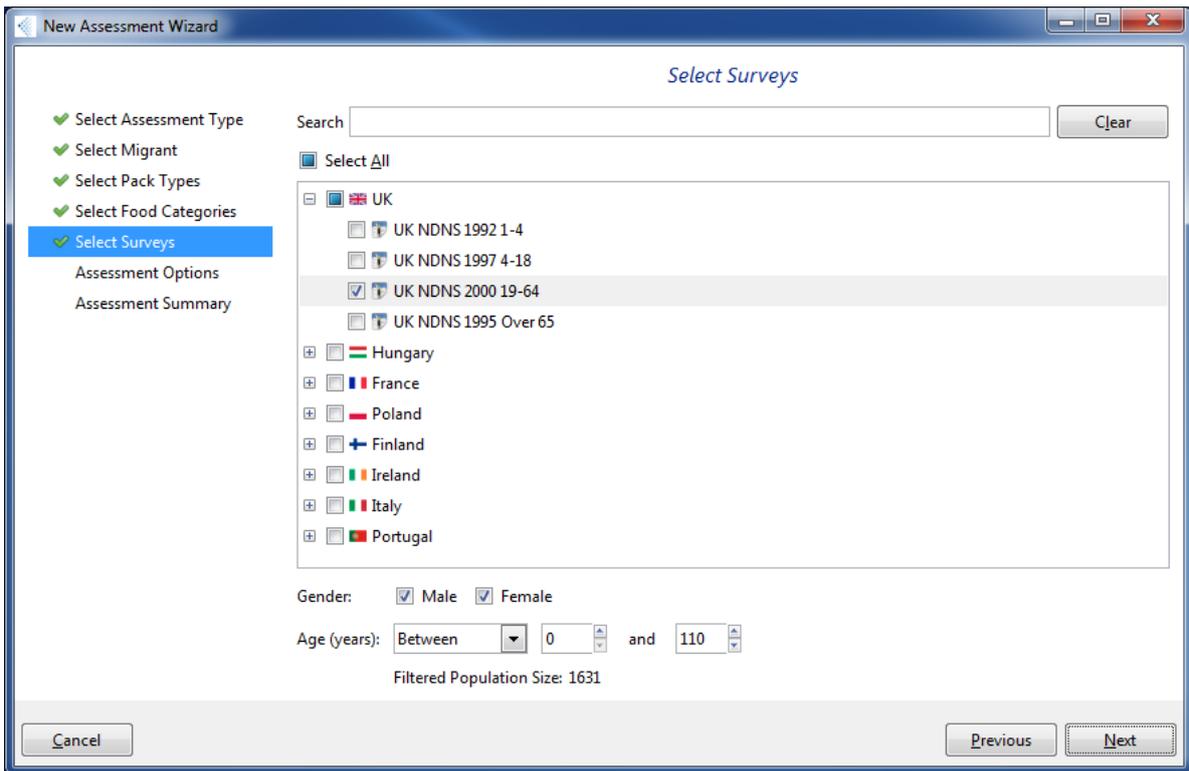


Figure 3-6: Selection of Survey

After the user has clicked “Next”, the user is now presented with various “Assessment Options”, as illustrated in Figure 3-7. These include the option to name the assessment, whether to assess using “consumer loyalty”, and the option to exclude homegrown or restaurant foods. These options are explained as part of this example.

There are other options to “Use SetOff” and more advanced options. These will be described and used at a later stage in the training.

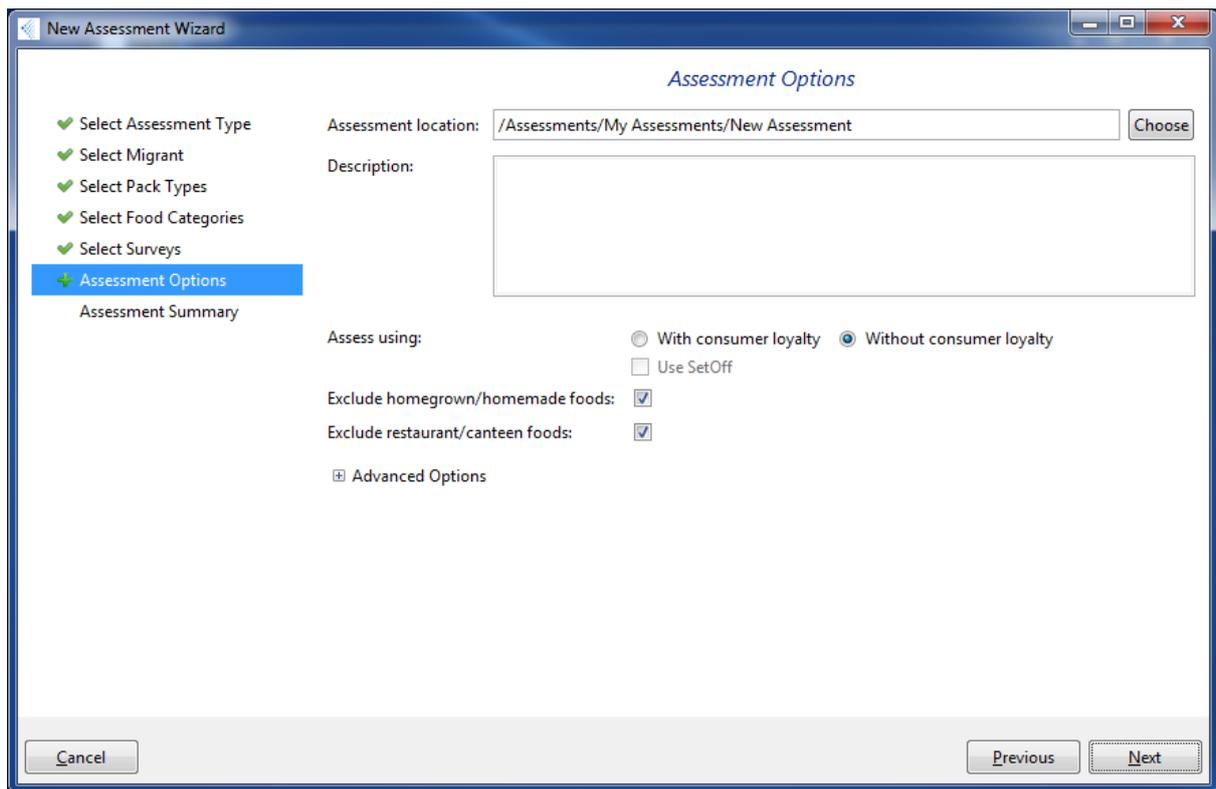


Figure 3-7: Selecting Options

One of the options mentioned above is giving a name to the assessment. When the user has completed many assessments, it is useful to have an assessment name that highlights the important information encoded in the assessment. To name an assessment requires the user to click the "Choose" button shown in Figure 3-7. This opens a window, as shown in Figure 3-8, where the user enters the appropriate assessment name and then clicks "Save". In this instance, name the assessment "Substance: 1084 – Survey: UK\_19-64"

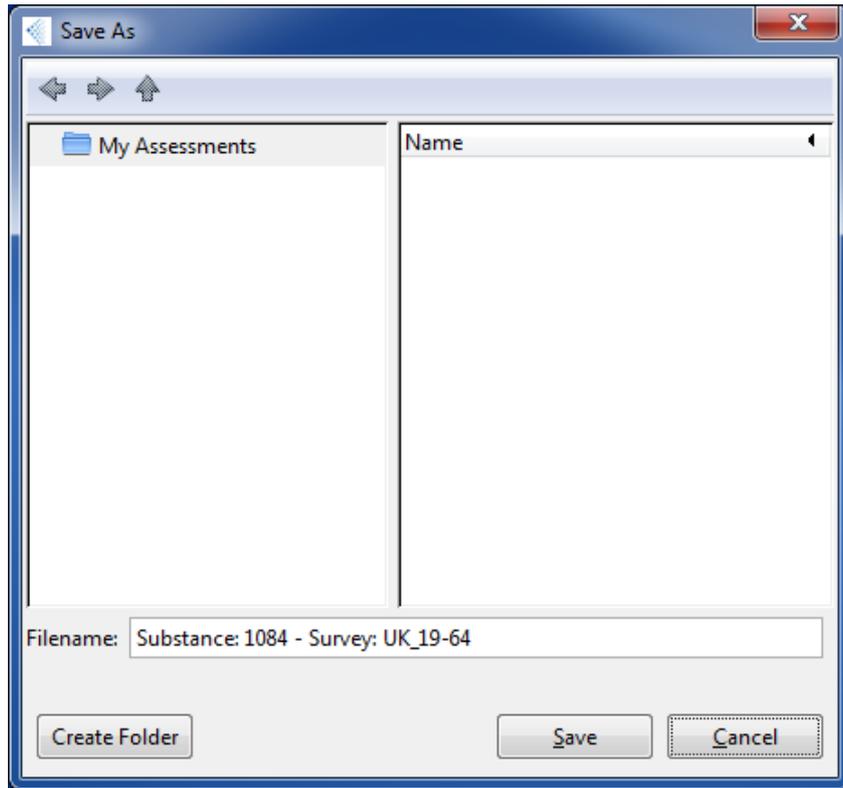


Figure 3-8: Naming the Assessment

Once a name has been given to the assessment, the name will be shown in the “Assessment Options” window, as illustrated in Figure 3-9. Also, select “Without consumer loyalty” and tick the “Exclude homegrown/homemade foods” and “Exclude restaurant/ canteen foods” boxes. Again, the user needs to click the “Next” button.

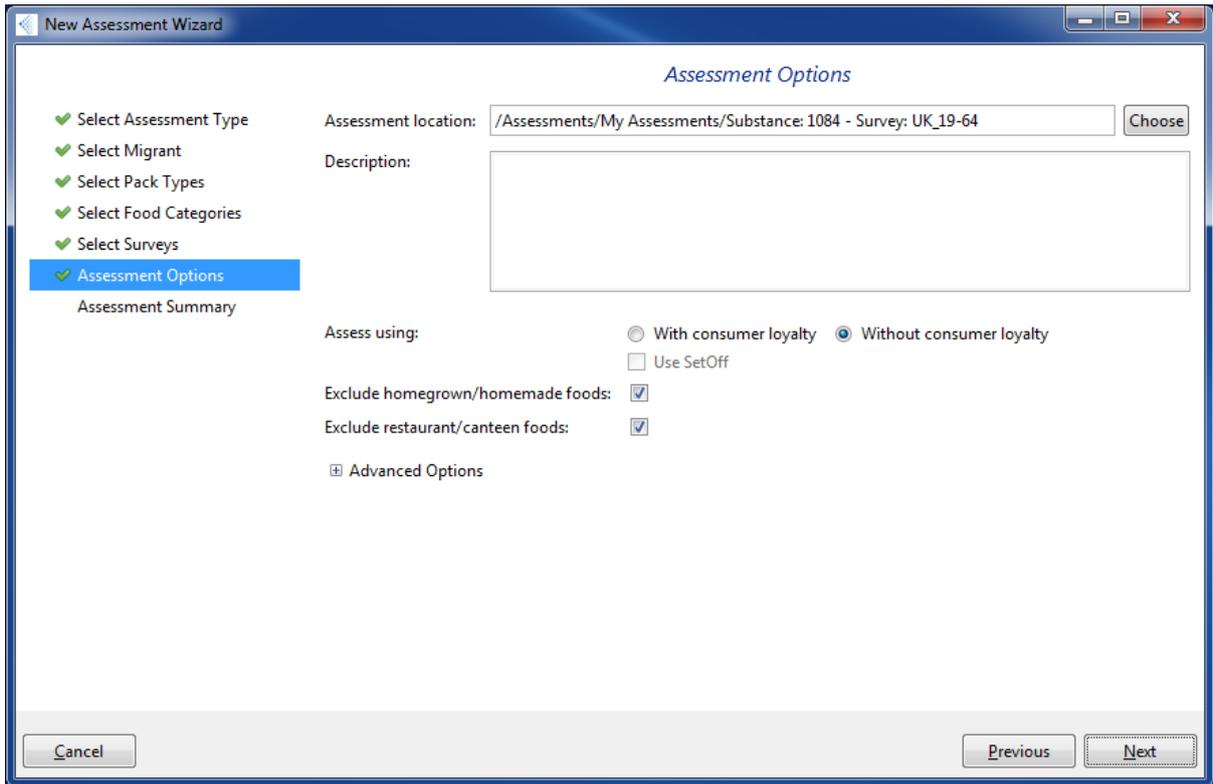


Figure 3-9: Checking Assessment Name

At this stage an “Assessment Summary” is provided. This is shown in Figure 3-10. If the user is happy with the details of the summary, the “Run” button is selected. This produces a window telling the user, as shown in Figure 3-11, that the assessment has been submitted. Click “OK”.

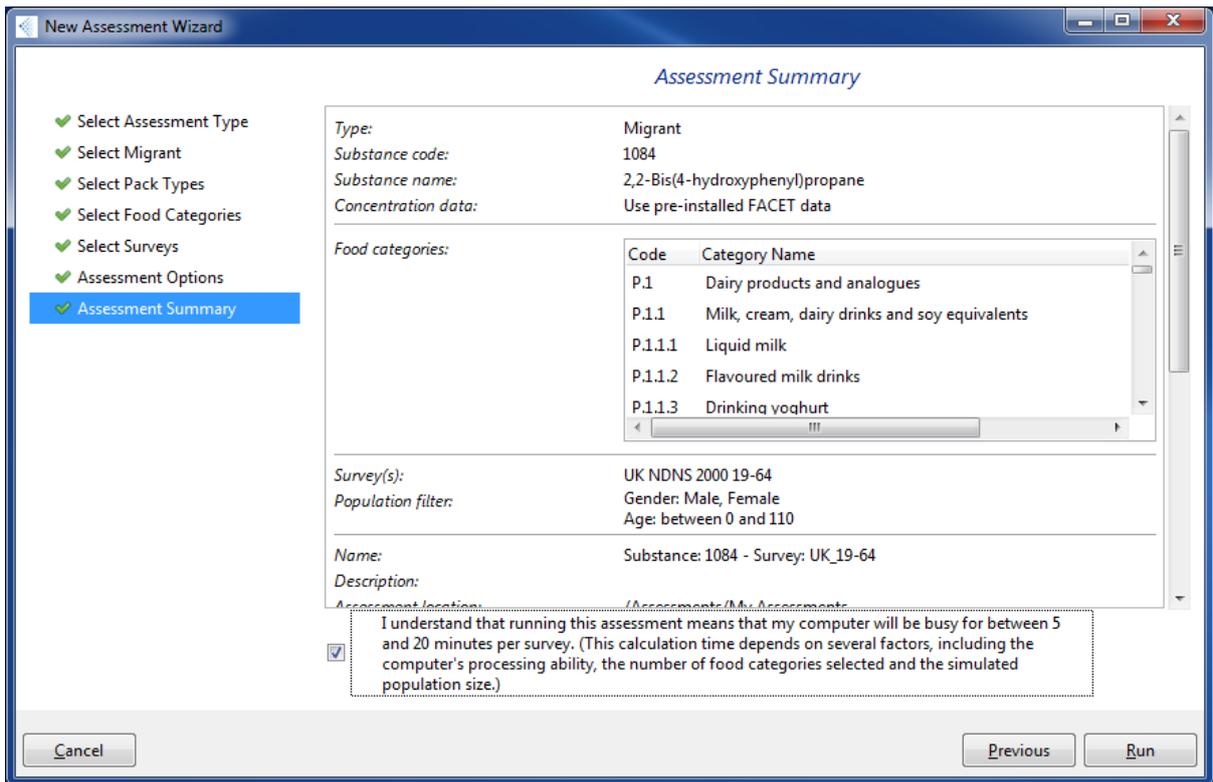


Figure 3-10: Summary of Assessment Before Run

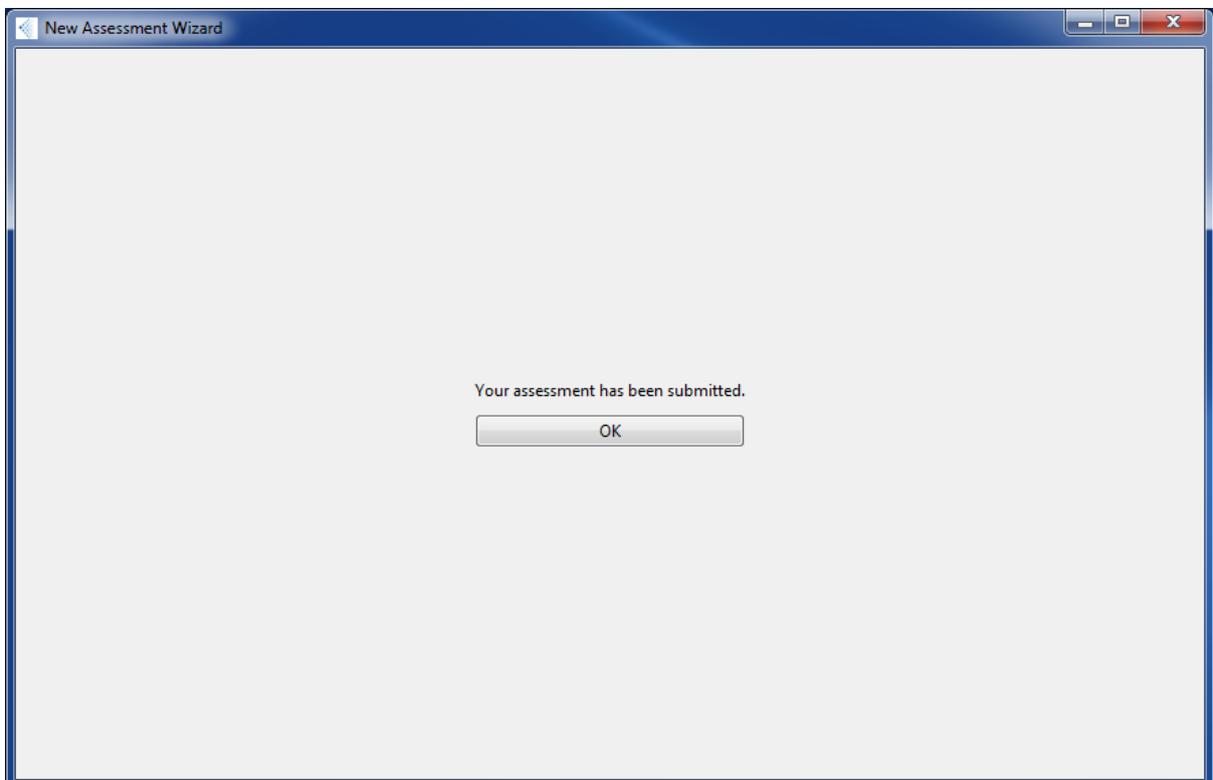


Figure 3-11: Assessment Submitted

The user should at this stage select “Assessments” and then “My Assessments” as is shown in Figure 3-12. Once the “Initialising” stage has finished, the assessment moves into the “Progress” stage. A progress bar is illustrated to inform the user of the percentage completion of the assessment. This is illustrated in Figure 3-13.

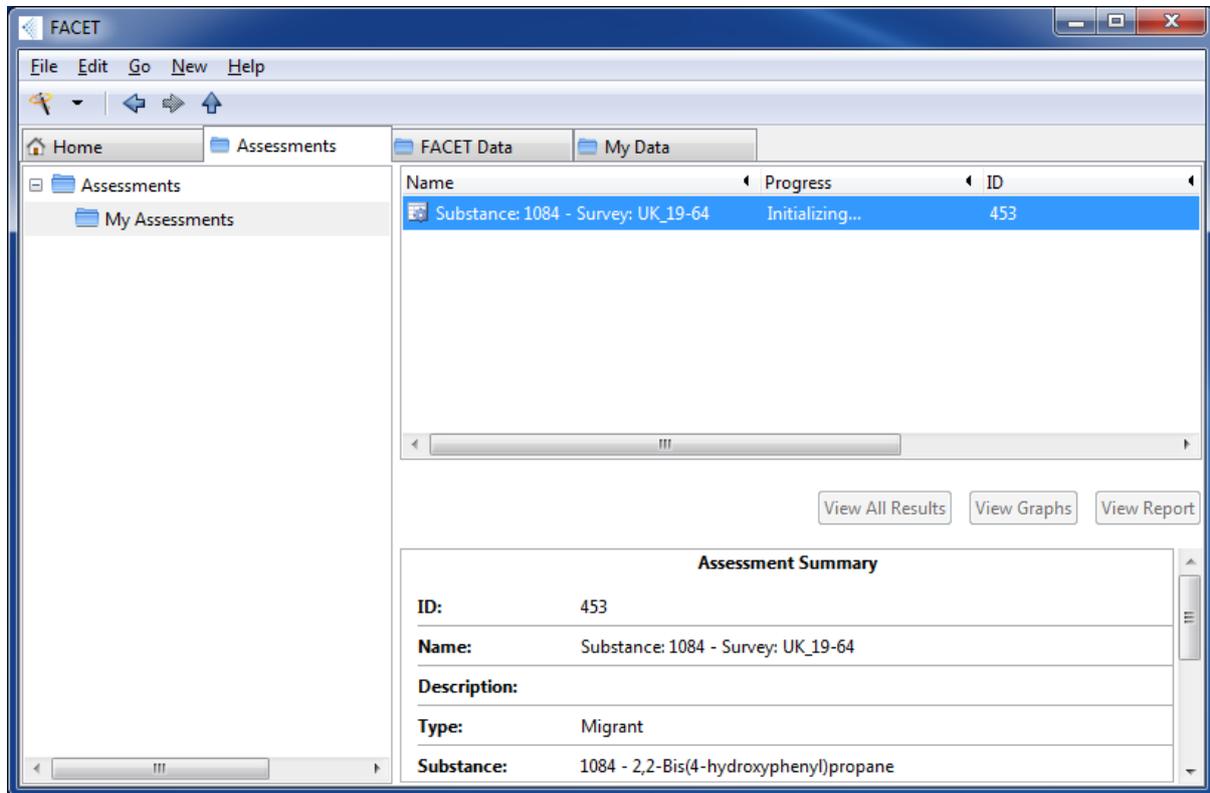


Figure 3-12: Assessment Initialising

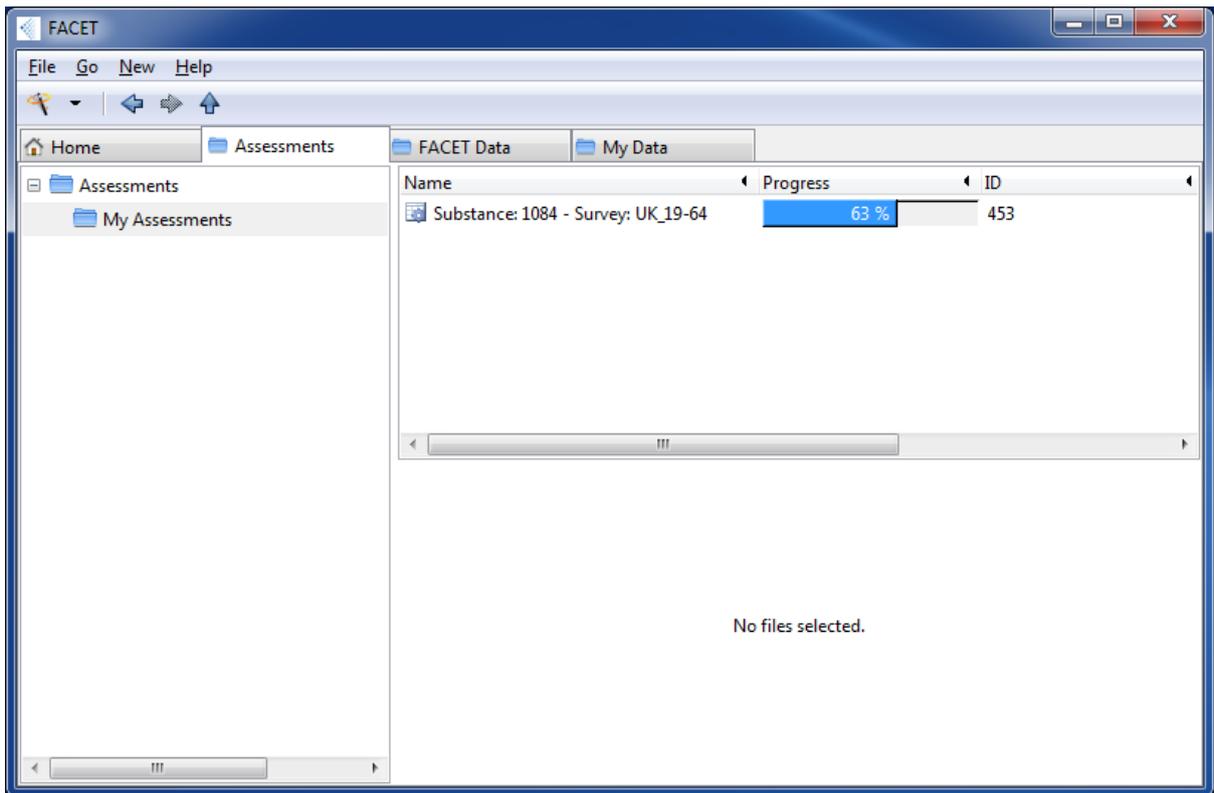


Figure 3-13: Assessment in Progress

Once the assessment completes, the user is informed of this with Progress set to “Complete”. This is shown in Figure 3-14.

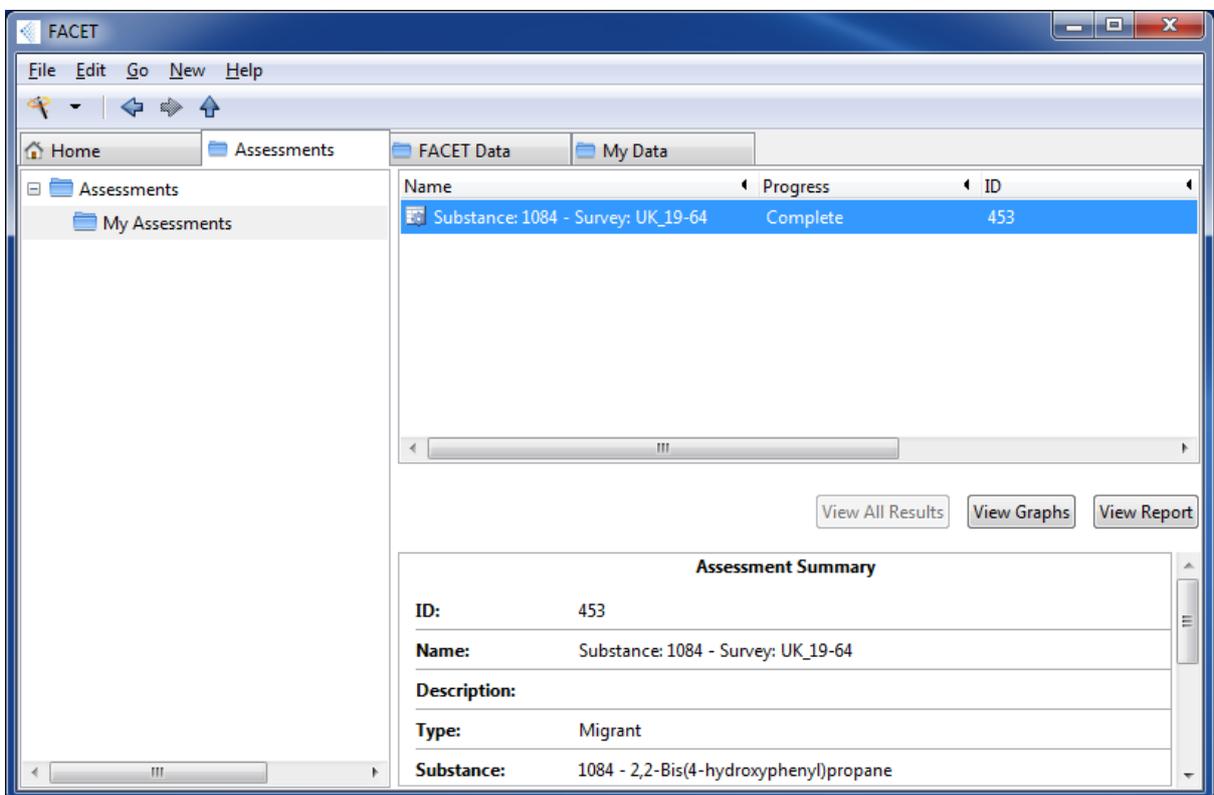


Figure 3-14: Assessment Complete

Once the assessment completes, the user can now access the results of the assessment. Before viewing the results (in Section 3.2), another useful option in the software can be explained. That is, the renaming of a table. To rename a table, the user initially selects the table, and then right clicks the mouse as illustrated in Figure 3-15. This gives the option to “Rename” or indeed “Delete” an assessment. To rename the assessment, select the “Rename” option. This has the effect of opening a pop-up window as shown in Figure 3-16.

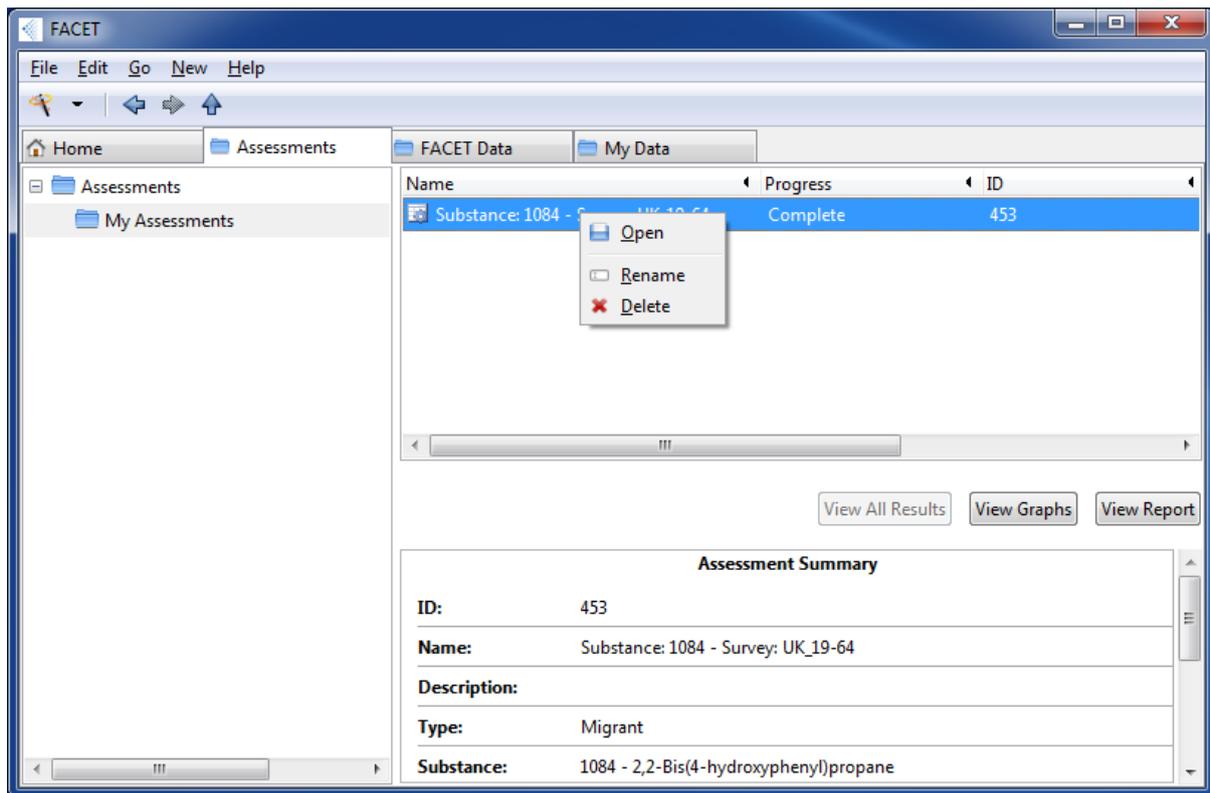


Figure 3-15: Rename Table

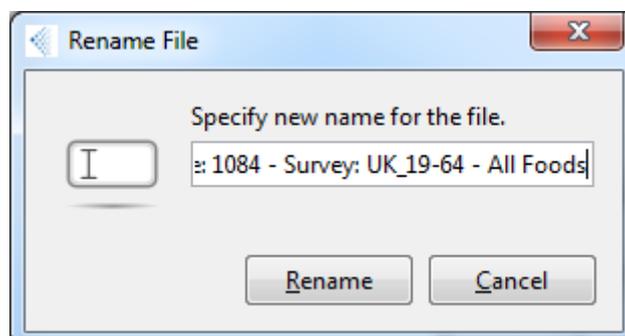
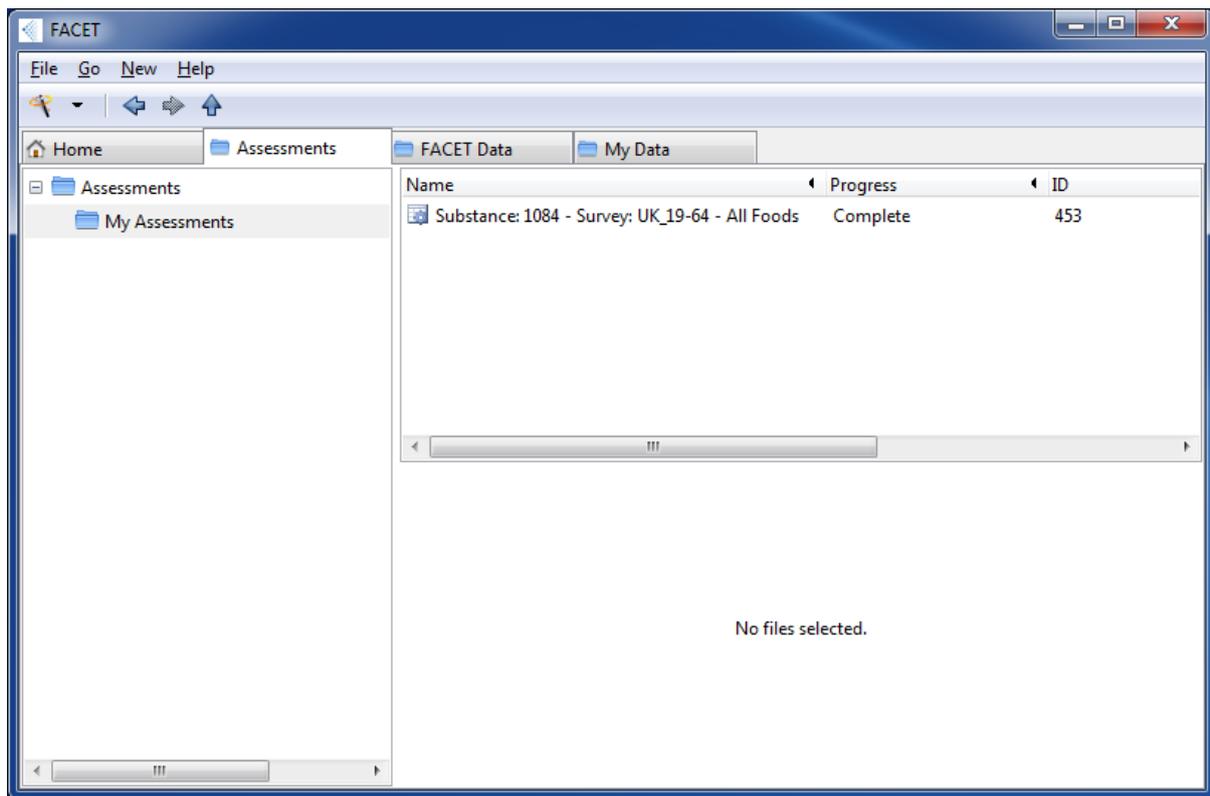


Figure 3-16: Renaming Table

At this stage the user can view the table and confirm its new name. This is shown in Figure 3-17.



The screenshot shows the FACET software interface. The window title is 'FACET'. The menu bar includes 'File', 'Go', 'New', and 'Help'. Below the menu bar are navigation icons. The interface is divided into several panes. On the left, there is a 'Home' pane with a tree view showing 'Assessments' and 'My Assessments'. The main area is split into two panes: 'FACET Data' and 'My Data'. The 'FACET Data' pane contains a table with the following data:

Name	Progress	ID
Substance: 1084 - Survey: UK_19-64 - All Foods	Complete	453

Below the table, there is a horizontal scrollbar. The 'My Data' pane is currently empty and displays the text 'No files selected.' at the bottom.

Figure 3-17: Table After Renaming

### 3.1.1 Exercises

#### Exercises for Basic Packaging Assessment

- (i) Run a Packaging Assessment satisfying the following criteria
  - a. Substance: 1084
  - b. Pack Types: All Pack Types
  - c. Foods: P.15 Alcoholic Beverages and P.18 Composite Foods
  - d. Survey: UK 19-64
  - e. Select Males between the ages of 20 and 25
  - f. Assessment Name: Substance: 1084 – Survey: UK\_19-64 – Packs: [P.15, P.18] – Foods: All – Loyal: Yes
  - g. Select “With consumer loyalty”

- (ii) Run a Packaging Assessment satisfying the following criteria
  - a. Substance: 1334
  - b. Pack Types: Main = Plastic Tray/ Pot/ Tub/ Cup  
 Closure = Sealed Lidding/ membrane, Plastic snap on lidding  
 Exclude Outer and Insert components
  - c. Foods: P.17.1.1 Spoonable yoghurt
  - d. Survey: UK 19-64
  - e. Males and Females between 0 and 110
  - f. Assessment Name: Substance: 1334 – Survey: UK\_19-64 – Packs: [Main, Closure] –  
 Foods: P.17.1.1 – Loyal: No
  - g. Select “Without consumer loyalty”

### 3.2 Examining Results

Once the assessment has completed, the user can access the results of the assessment. This can be done in two ways: “View Graphs” and “View Report” as shown in Figure 3-18.

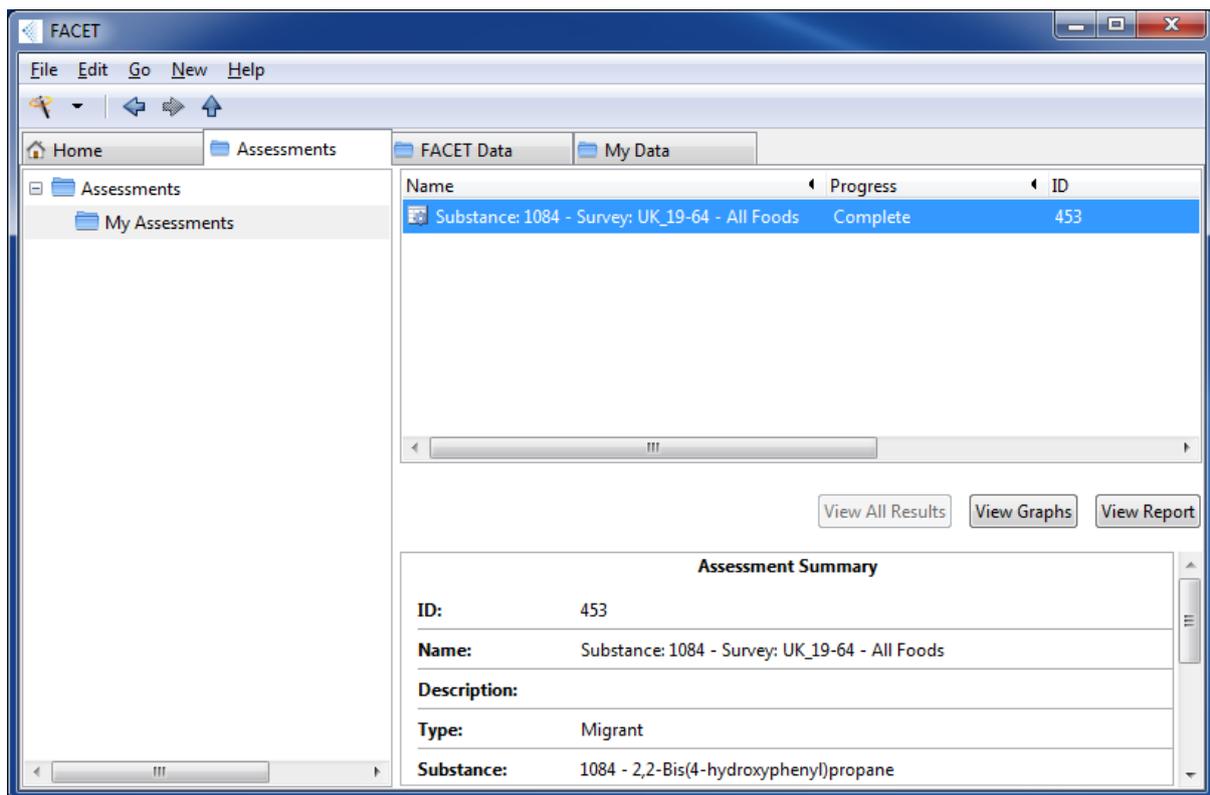


Figure 3-18: Viewing Results

If the user selects the “View Report” option then a report is displayed. For this example, the report is shown in Figure 3-19 and Figure 3-20.

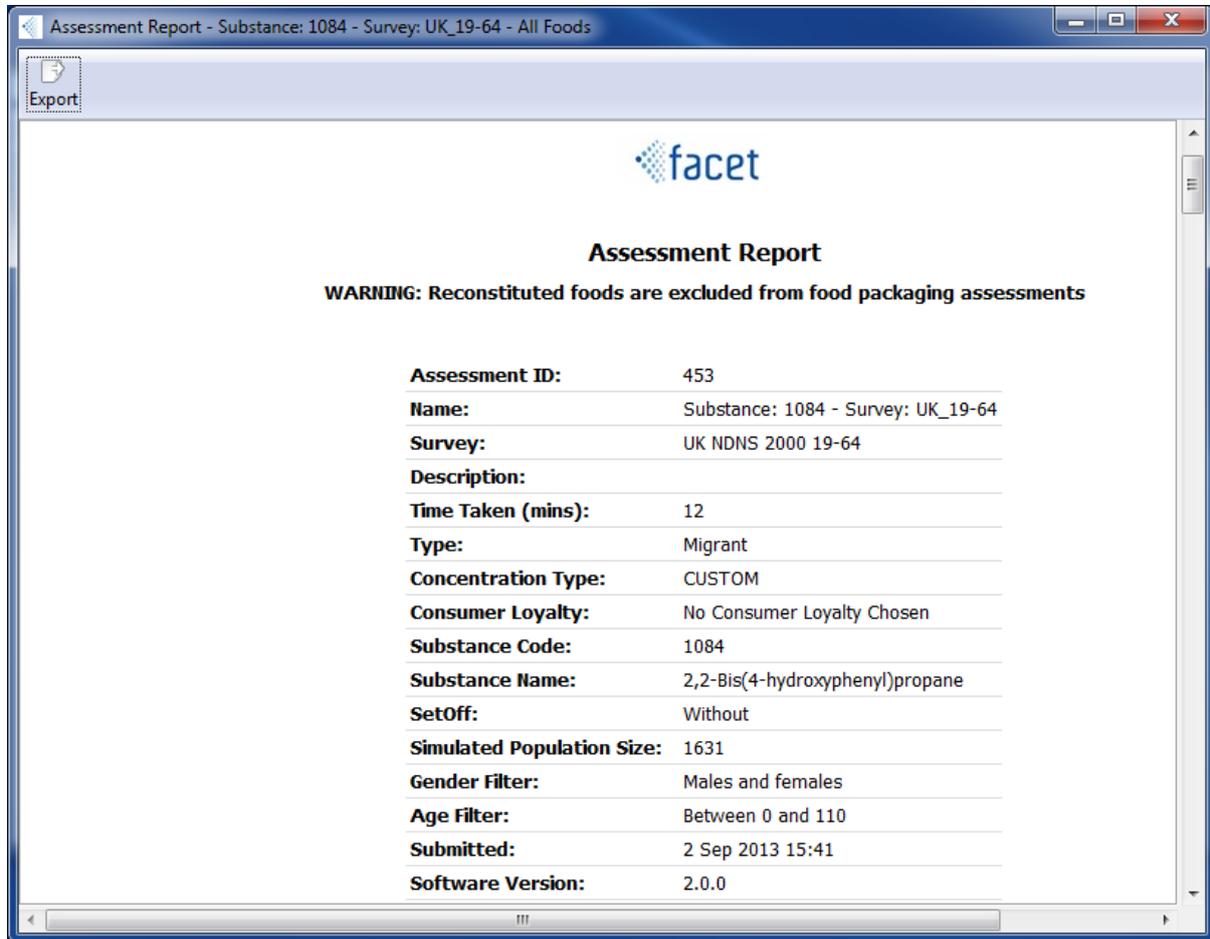


Figure 3-19: Assessment Report (Inputs)

Assessment Report - Substance: 1084 - Survey: UK\_19-64 - All Foods

Export

**2,2-Bis(4-hydroxyphenyl)propane - All Pack Types - Exposure, Absolute, Total Population (mg/d)**

Food Category	Count*	Mean	P90	P95
P.11 - Sweeteners and honey	1631	5.284e-6 ± 9.25e-7	0 ± 0	0.00001318 ± 4.415e-6
P.12 - Salt, spices, herbs, sauces and soups	1631	0.0007093 ± 0.00005179	0.002255 ± 0.0002317	0.00413 ± 0.0002657
P.3 - Fruits, nuts and seeds	1631	0.0002468 ± 0.00003093	0.0003959 ± 0.00004906	0.001168 ± 0.0001488
P.4 - Vegetables, starchy roots, legumes and seaweeds	1631	0.0007235 ± 0.00004303	0.002111 ± 0.000148	0.003436 ± 0.0002091
P.10 - Eggs and egg products	1631	0 ± 0	0 ± 0	0 ± 0
P.6 - Cereals and cereal products	1631	0 ± 0	0 ± 0	0 ± 0
P.5 - Chocolate products and confectionery	1631	0 ± 0	0 ± 0	0 ± 0
P.13 - Nutritional foodstuffs	1631	0 ± 0	0 ± 0	0 ± 0
P.8 - Meat and meat products	1631	0.00008011 ± 0.00001327	0 ± 0	0.0002916 ± 0.00008437
P.14 - Non-alcoholic beverages (except dairy beverages)	1631	0.001704 ± 0.0001067	0.005382 ± 0.0006895	0.01004 ± 0.0008584
P.16 - Ready-to-eat savouries	1631	0 ± 0	0 ± 0	0 ± 0

Figure 3-20: Assessment Report (Statistics)

The report itself can be exported to a .csv file by clicking the “Export” button at the top left of the report as shown in Figure 3-21.

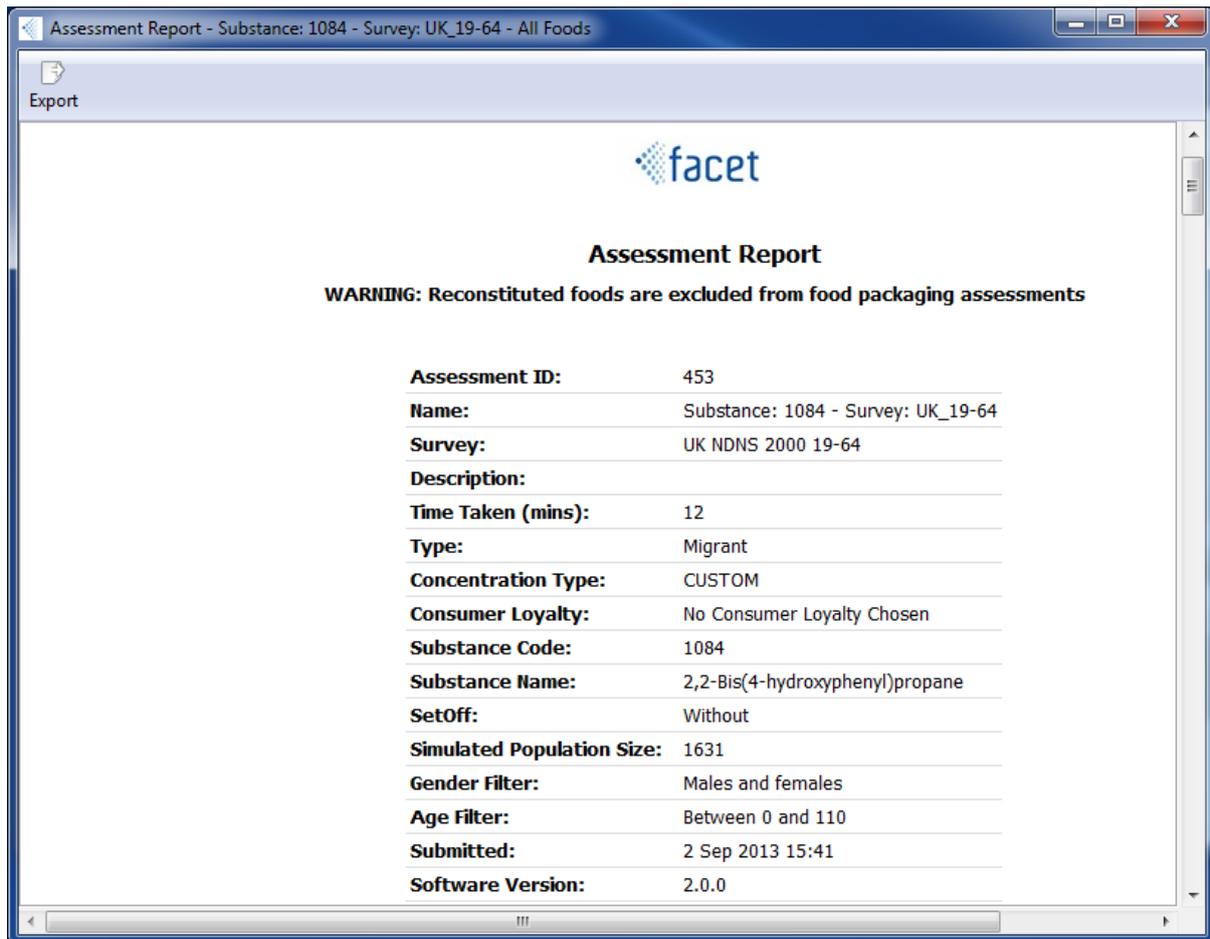


Figure 3-21: Exporting the Report

As well as viewing the numerical data outputted from the assessment, another option is to view graphs arising from the data. This is possible by clicking the “View Graphs” button as illustrated in Figure 3-22.

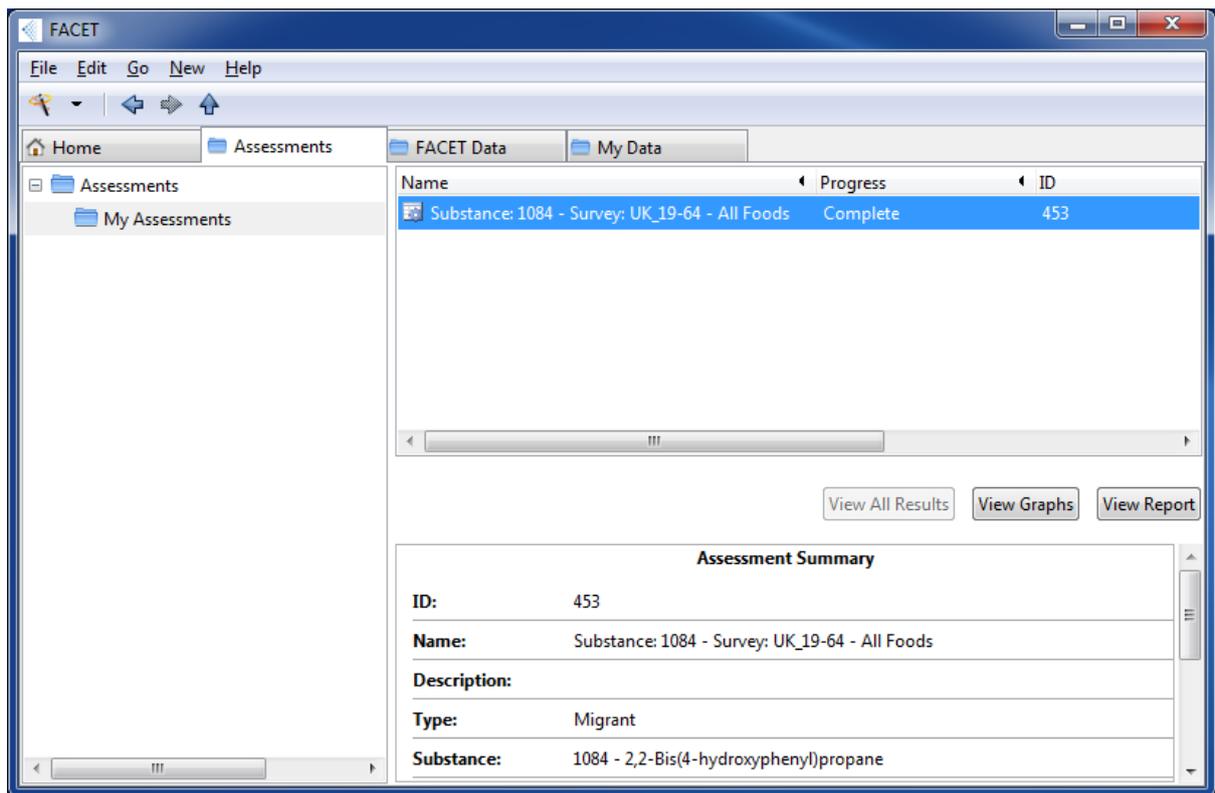


Figure 3-22: View Graphs

The graphs can be viewed “By Pack Type” or “By Food Category”. Initially the “By Pack Type” option will be described.

Selecting the “By Pack Type” option displays two bar charts as well as the numerical statistical data arising from the assessment. This is shown in Figure 3-23. The first bar chart illustrates the mean chemical exposure to the chosen substance (i.e. BPA) for “Total Population” while the second bar chart shows the chemical exposure to BPA for “Food Consumers”.

There are further options to filter the data placed under the bar charts. For example, instead of displaying the data for the “Per unit body weight” Intake Type, the user can select “Absolute”. This has the effect of changing the data to match the appropriate Intake Type (i.e. Absolute) as well as re-graphing the bar charts to match the updated data. This is shown in Figure 3-24.

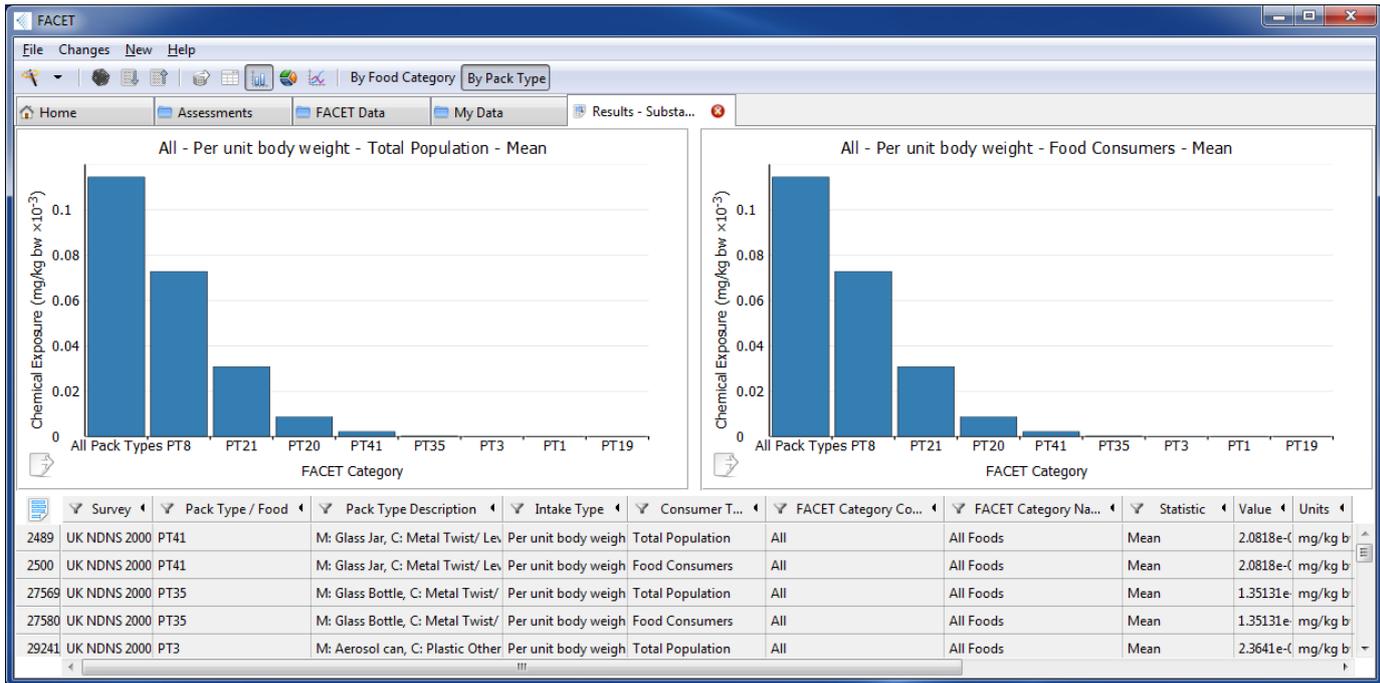


Figure 3-23: Graphs (By Pack Type), Column charts

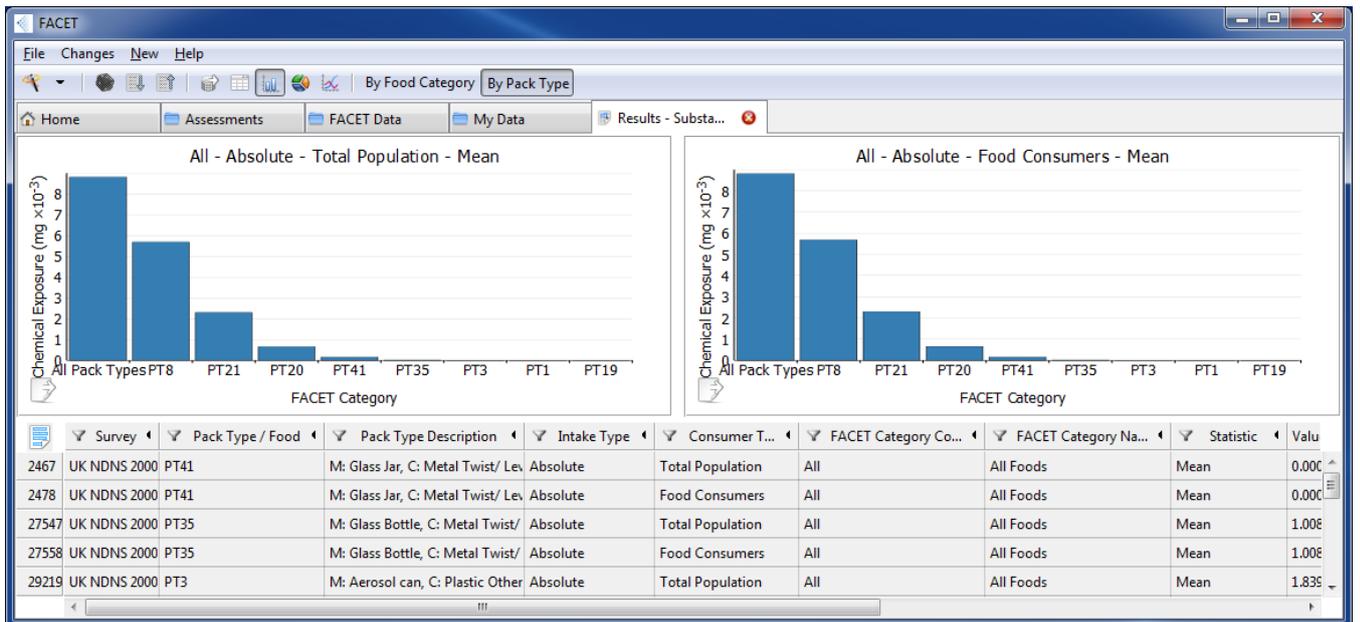


Figure 3-24: Filtering the Data

As well as viewing data using bar charts, a second option is to use pie charts. This option is possible by clicking the coloured disk/pie at the top of the window illustrated in Figure 3-25.

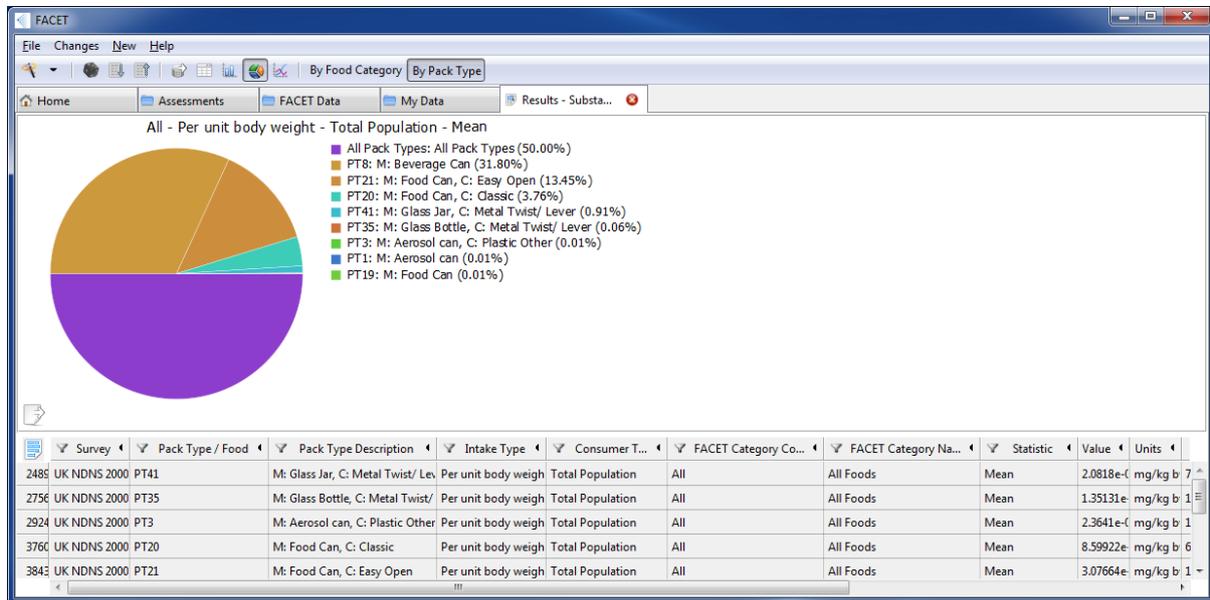


Figure 3-25: View Graphs (By Pack Type), Pie Chart

Also, the user has the option to filter the outputs of the assessment. For example, the Intake type can be change from “Per unit body weight” to “Absolute” as earlier. This will have the effect of updating the numerical statistical data as well as the associated graph (i.e. pie chart in this case). This shown in Figure 3-26.

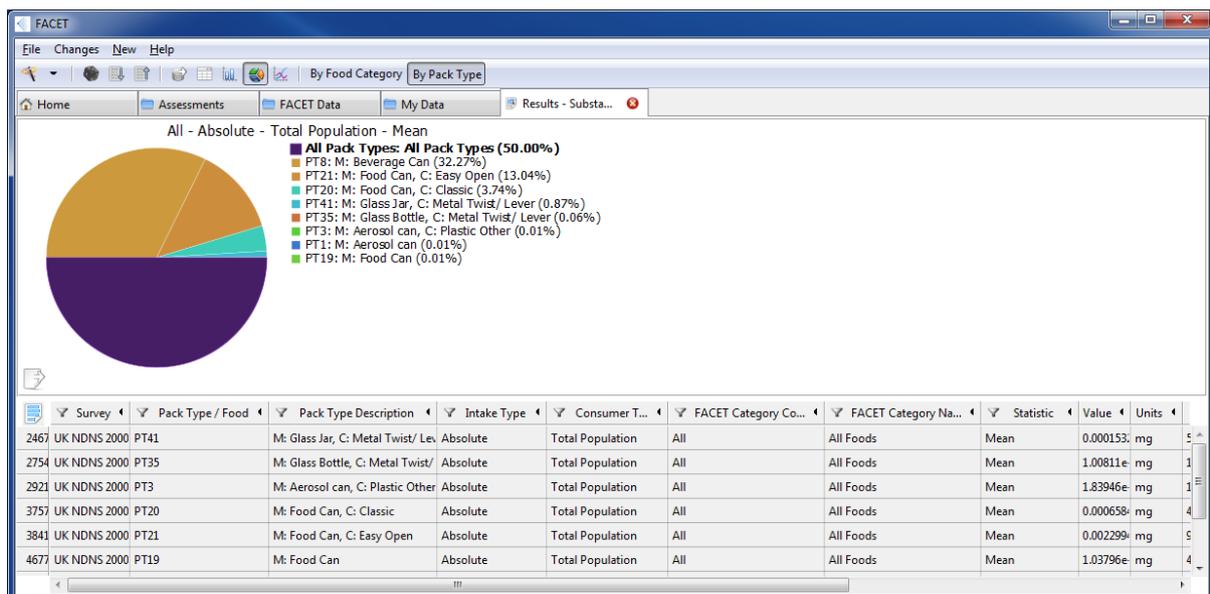


Figure 3-26: Filtering the Data

Instead of examining the assessment outputs “By Pack Type” the user can alternatively view the results “By Food Category”. This is made possible by clicking the “By Food Category” button as shown in Figure 3-27.

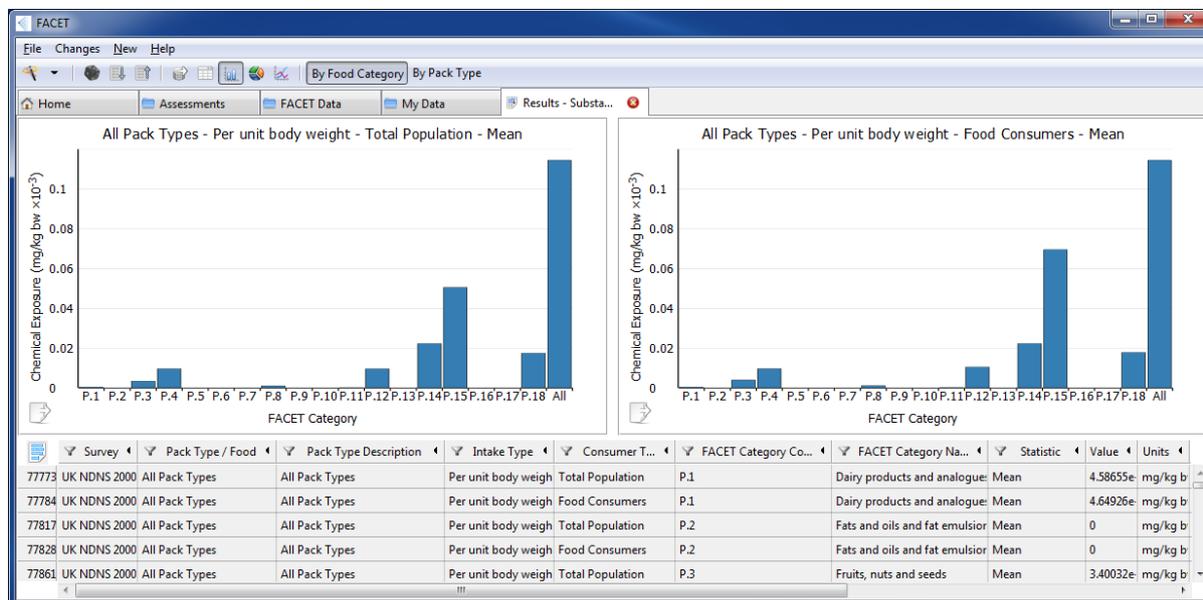


Figure 3-27: View Graphs (By Food Category), Column Charts

As with the option “By Pack Type” the user can also view the “By Food Category” data using pie charts. This option is illustrated in Figure 3-28.

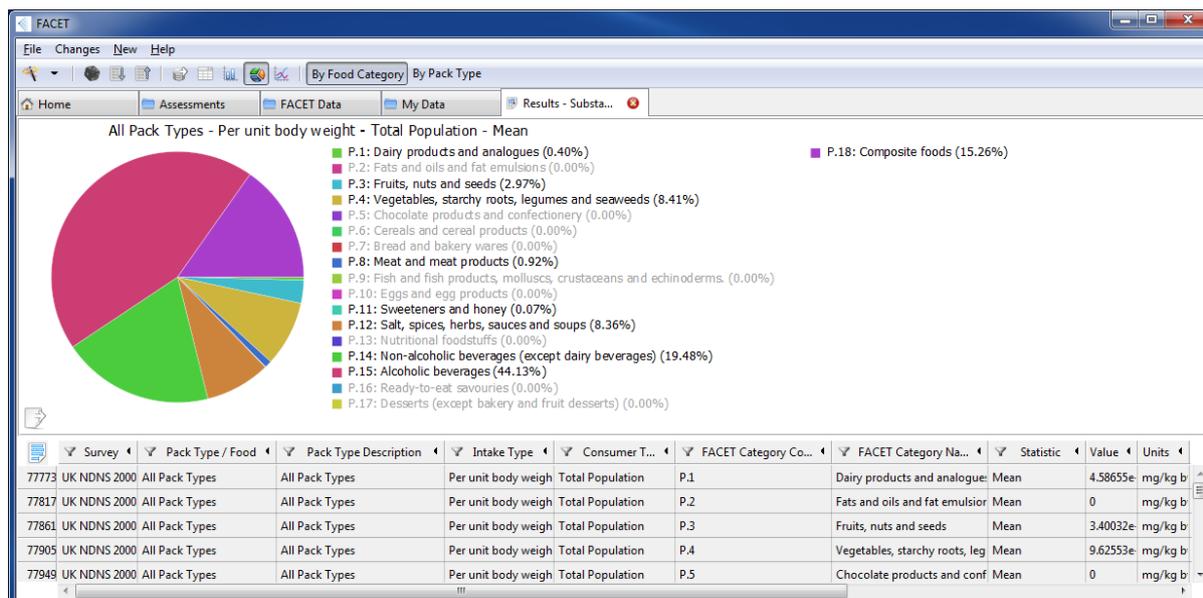


Figure 3-28: View Graphs (By Food Category), Pie Chart

The statistical data can be viewed without the use of graphs also. To do this, click the spreadsheet button at the top of the window in Figure 3-29.

	Survey	Pack Type / Food	Pack Type Description	Intake Type	Consumer T...	FACET Category Co...	FACET Category Na...	Statistic	Value	Units
1	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Total Population	P.1	Dairy products and analogue:	Count	1631	
2	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Total Population	P.1	Dairy products and analogue:	Percentage Consu	100	%
3	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Total Population	P.1	Dairy products and analogue:	Mean	0	mg
4	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Total Population	P.1	Dairy products and analogue:	Standard Deviatio	0	mg
5	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Total Population	P.1	Dairy products and analogue:	Minimum	0	mg
6	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Total Population	P.1	Dairy products and analogue:	Maximum	0	mg
7	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Total Population	P.1	Dairy products and analogue:	P25	0	mg
8	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Total Population	P.1	Dairy products and analogue:	P90	0	mg
9	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Total Population	P.1	Dairy products and analogue:	P95	0	mg
10	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Total Population	P.1	Dairy products and analogue:	CDF	Distributi	mg
11	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Total Population	P.1	Dairy products and analogue:	PDF	Distributi	mg
12	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Food Consumers	P.1	Dairy products and analogue:	Count	1609	
13	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Food Consumers	P.1	Dairy products and analogue:	Percentage Consu	98.6511	%
14	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Food Consumers	P.1	Dairy products and analogue:	Mean	0	mg
15	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Food Consumers	P.1	Dairy products and analogue:	Standard Deviatio	0	mg
16	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Food Consumers	P.1	Dairy products and analogue:	Minimum	0	mg
17	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Food Consumers	P.1	Dairy products and analogue:	Maximum	0	mg
18	UK NDNS 2000	PT33	M: Glass Bottle, C: Crimped alu	Absolute	Food Consumers	P.1	Dairy products and analogue:	P25	0	mg

Figure 3-29: Data Only

Finally, the user can export the graphs to a .png image to be used, for example, in a report. To do this the user chooses the “Export graph to local file” option. This is the button at the bottom left of the graph to be exported. This is shown in Figure 3-30. To export the data, the user selects “File” followed by “Export Data” as seen in the top left corner of Figure 3-30.

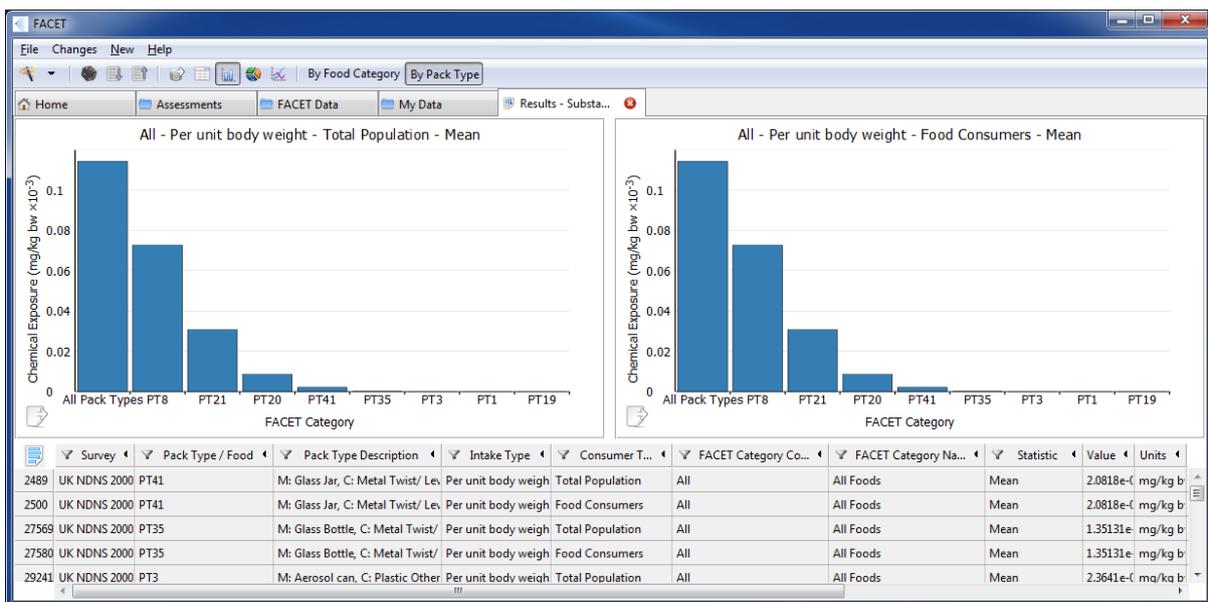


Figure 3-30: Export Graph to PNG image

### 3.2.1 Exercises: Examining Results

1. In the first exercise of Section 3.1.1 the assessment “Substance: 1084 – Survey: UK\_19-64 – Packs: [P.15, P.18] – Foods: All – Loyal: Yes” was created. Using the outputs from this assessment complete the following tasks.
  - a. Download the bar chart broken down “By Food Category” described as follows: “Per unit body weight” for “Total Population”
  - b. Download the bar chart broken down “By Food Category” described as follows: “Per unit body weight” for “Food Consumers”
  - c. Download the data broken down “By Food Category”
  - d. Download the pie chart broken down “By Food Category” described as follows: “Per unit body weight” for “Total Population”
  - e. Download the bar chart broken down “By Pack Type” described as follows: “Per unit body weight” for “Total Population”
  - f. Download the Report summarising the assessment outputs.

### 3.3 Entering extraction/migration data

Sometimes the user needs to run specific assessments based on the results of a survey. Another requirement may be to enter a new substance and run an exposure assessment for the substance under particular conditions. These types of assessments are possible using the “New Packaging Wizard”.

#### 3.3.1 Using the New Packaging Wizard for a Substance in a Metal Pack Type

The “New Packaging Wizard” is made available for use by selecting this option as shown in Figure 3-31.

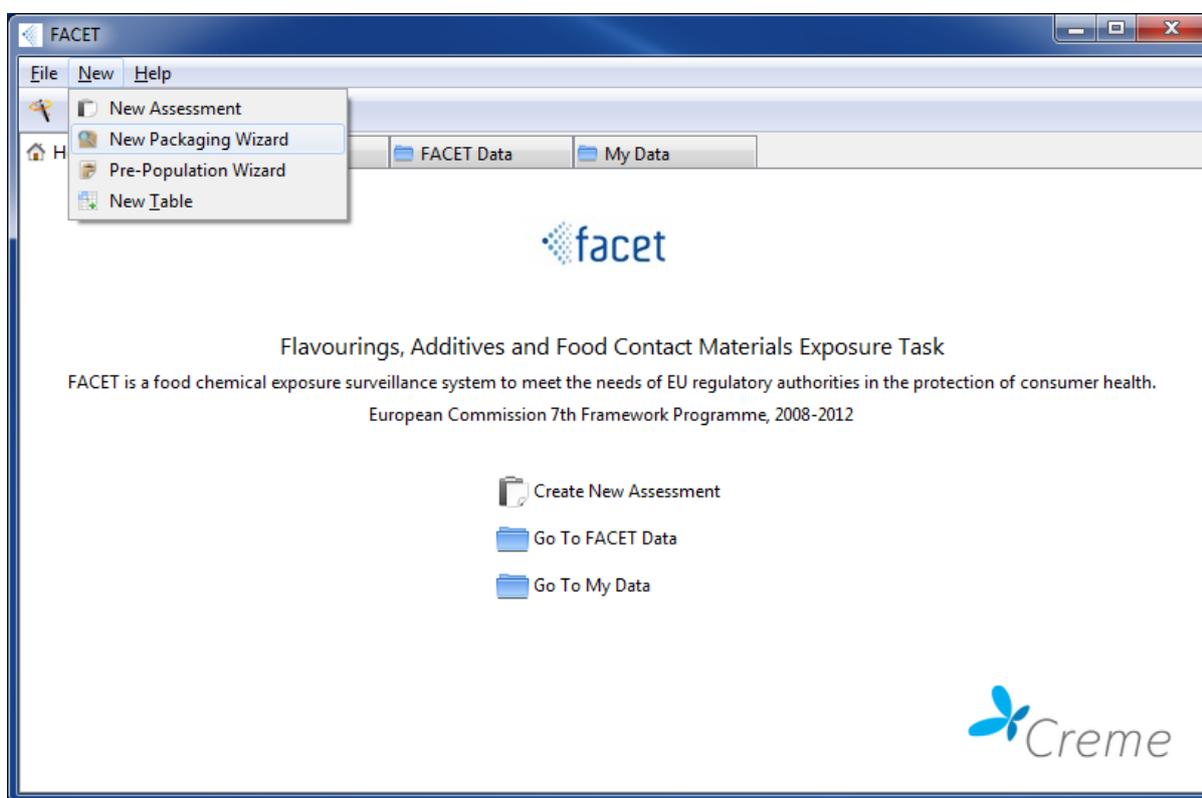


Figure 3-31: Select New Packaging Wizard

At this point, the user has two options. They can consider a substance in a pack type which is “Non-Metal” or “Metal”. For our example, we will select “New Metal Pack Type” as illustrated in Figure 3-32.

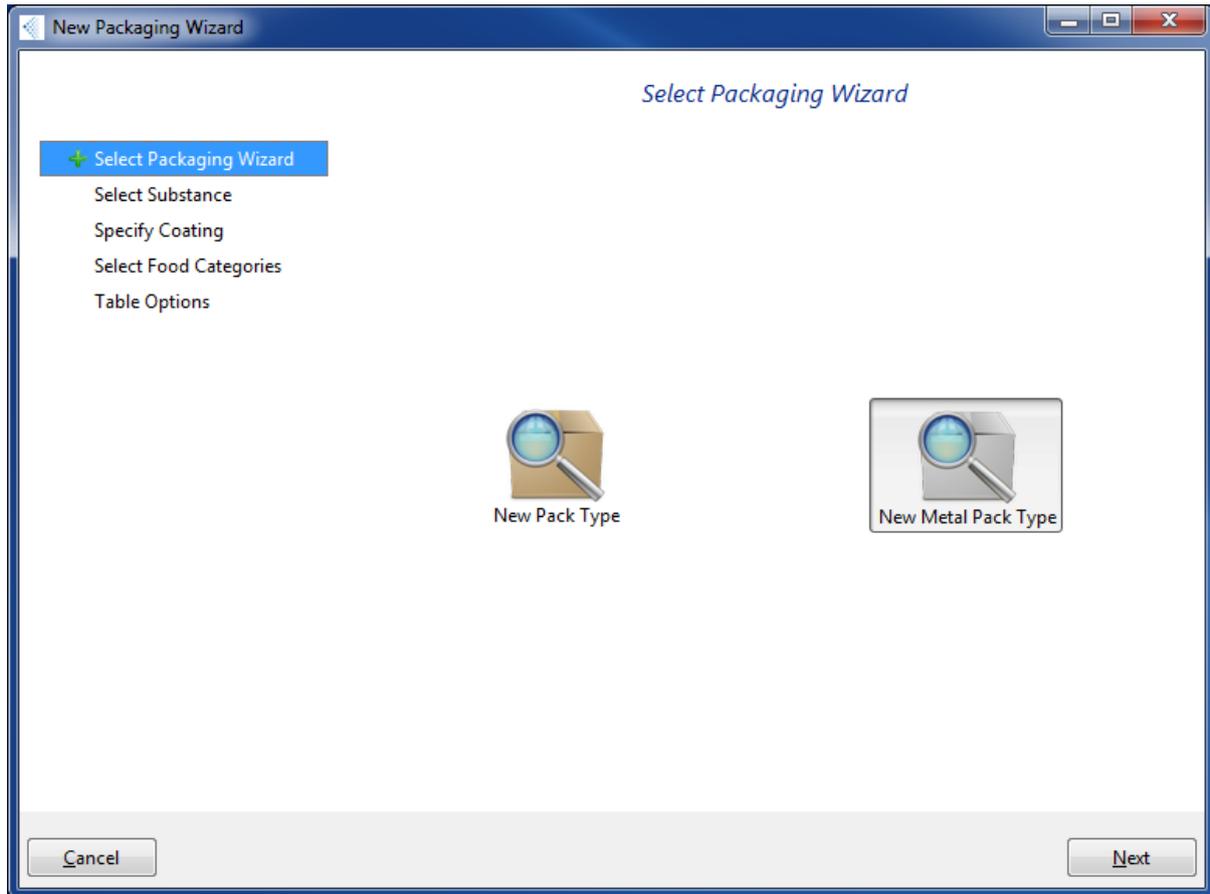


Figure 3-32: Select New Metal Pack Type

There is another choice at the next stage of the assessment. The user can select a “New Substance” or an “Existing Substance”. For this example, we select an “Existing Substance” called Styrene as shown in Figure 3-33.

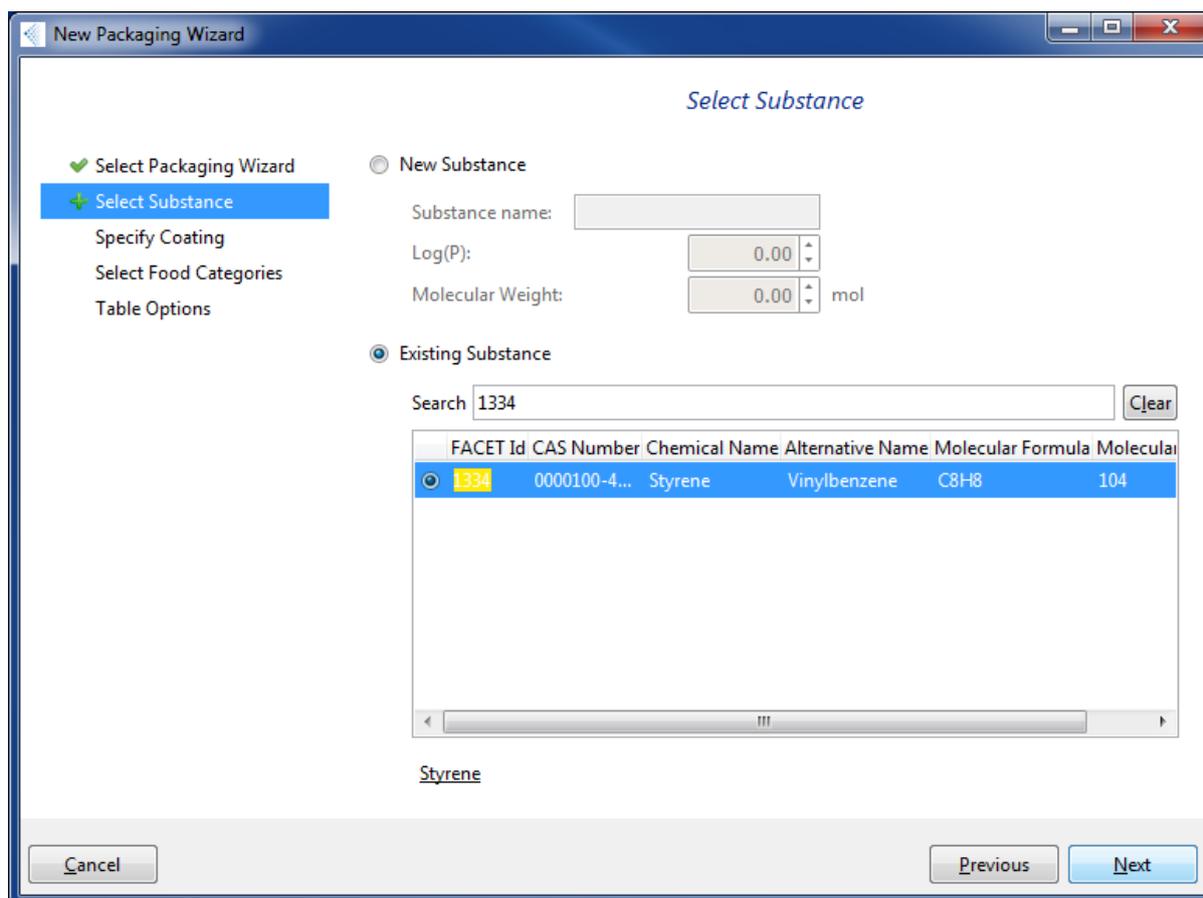


Figure 3-33: Select Existing Substance

At the next stage, the user can describe the details of the pack by selecting the Surface to Volume ratio, Pack Type, and Material Code. This process is illustrated in Figure 3-34 to Figure 3-39. In Figure 3-34 the Surface to Volume (ratio) is chosen. In our example, we use a Surface to Volume Ratio of  $0.6 \text{ cm}^2/\text{g}$ .

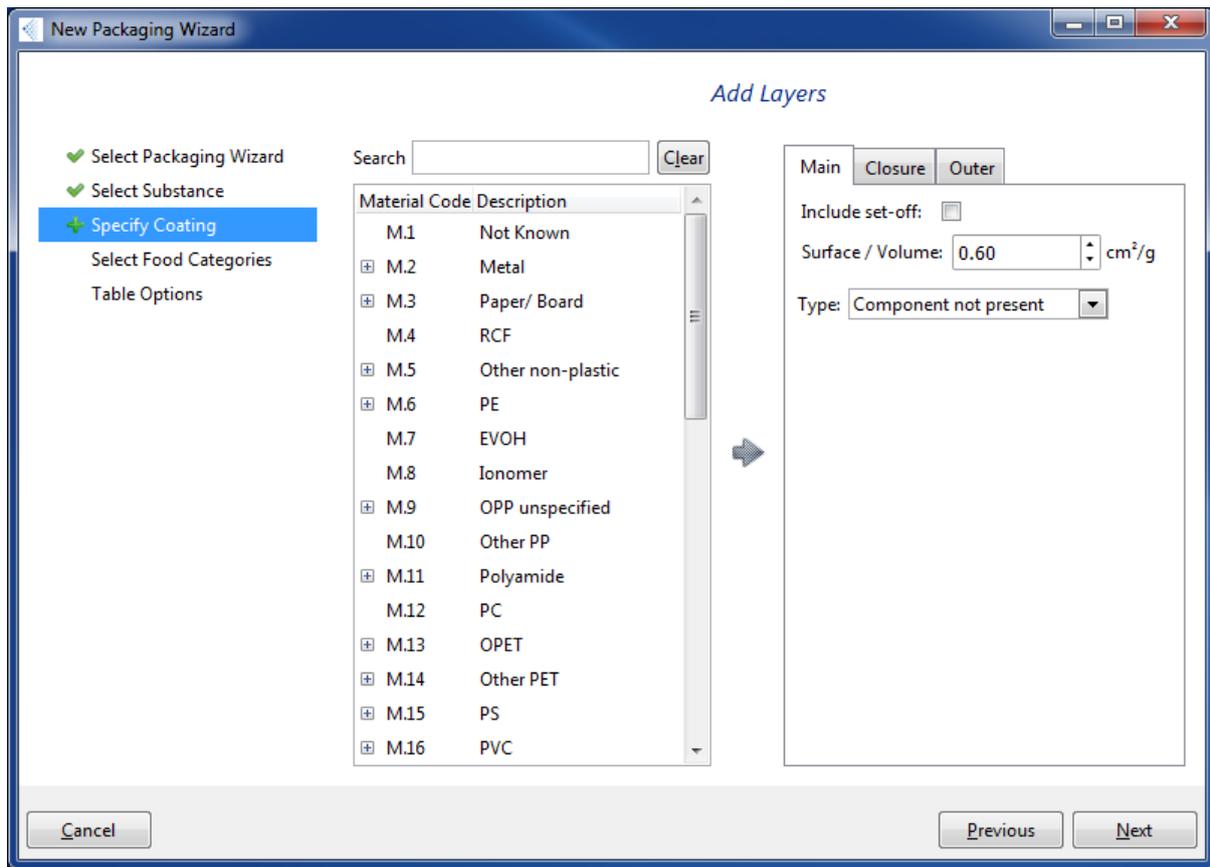


Figure 3-34: Select Surface/Volume

Next the (Pack) Type is selected. This is shown in Figure 3-35 where Beverage Can is the “Type” chosen.

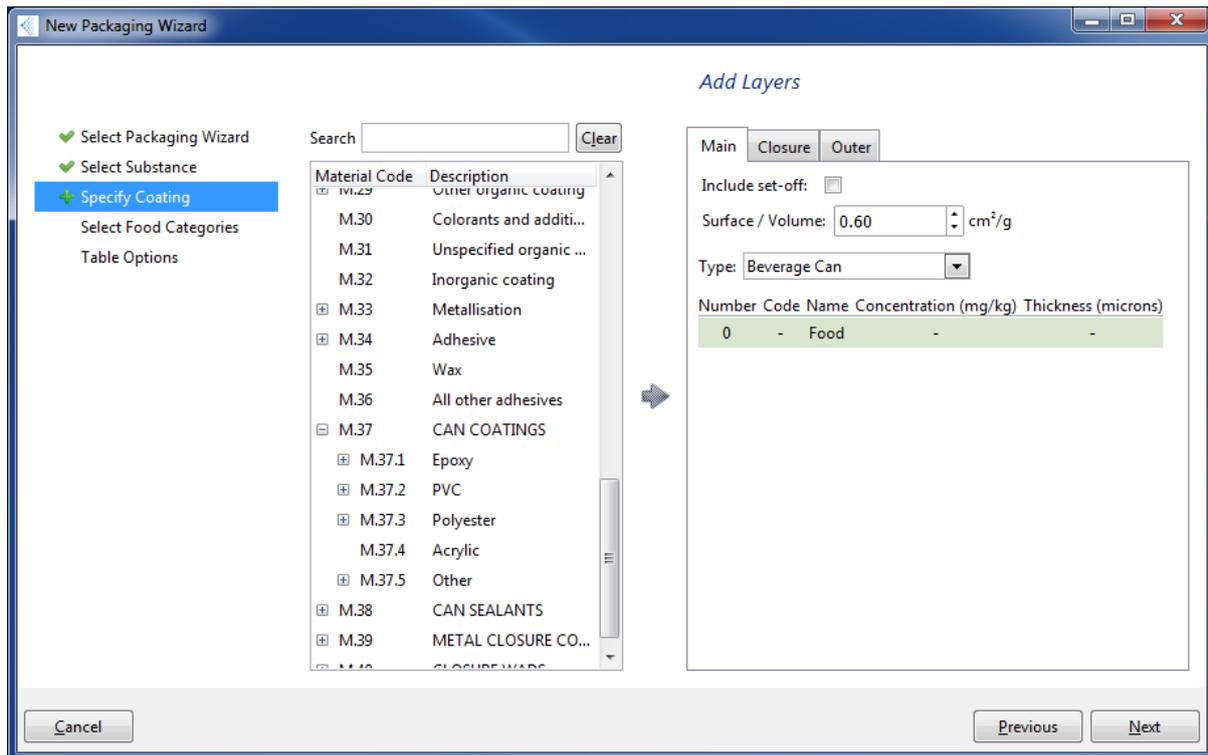


Figure 3-35: Select Pack Type

At this stage the user selects the materials/layers of the Pack Type. This is carried out by selecting the appropriate material. This step is shown in Figure 3-36 to Figure 3-39 where the material “M.37.1.4.1” is chosen. Initially, in Figure 3-36, an attempt is made to locate the required “Material Code”. This brings us to the “Material Code” M.37.1. The user will observe at this point that the “Material Code” is not fully visible. To resolve this, the user need to widen the “Material Code” field. This is done by clicking on the bar between “Material Code” and “Description” and moving the mouse to the right while the mouse remains clicked.

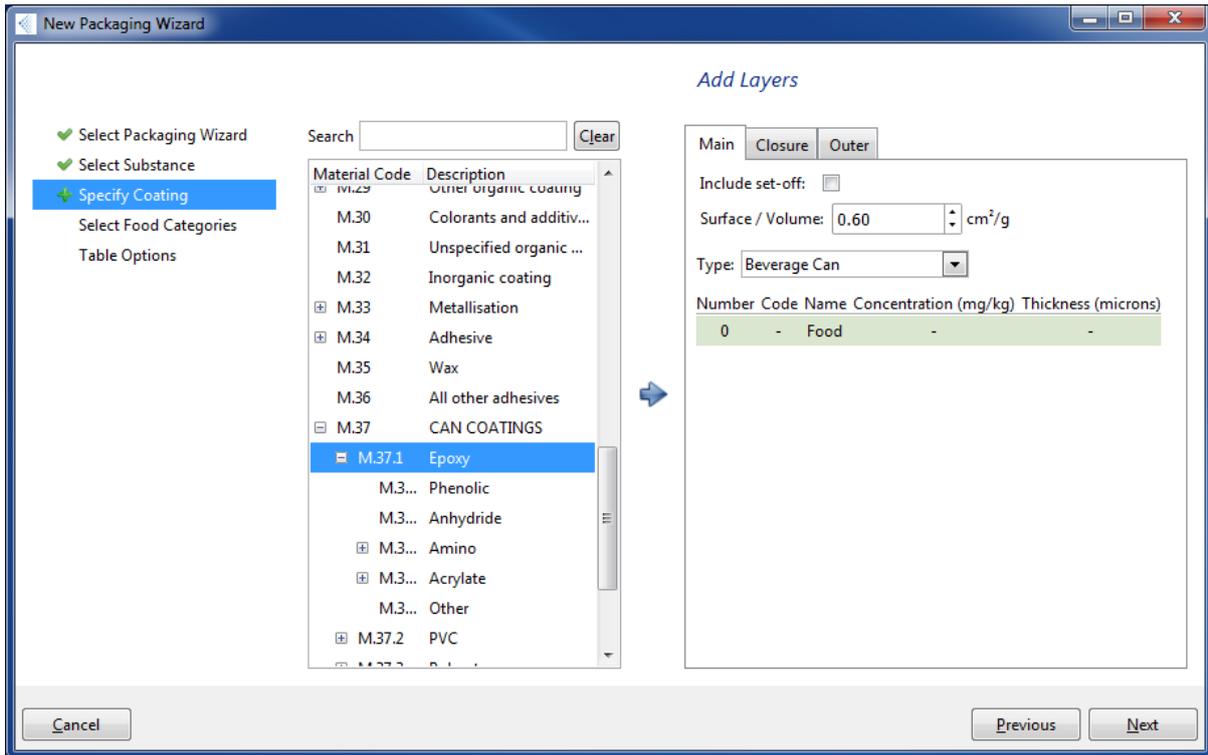


Figure 3-36: Searching for Material Code

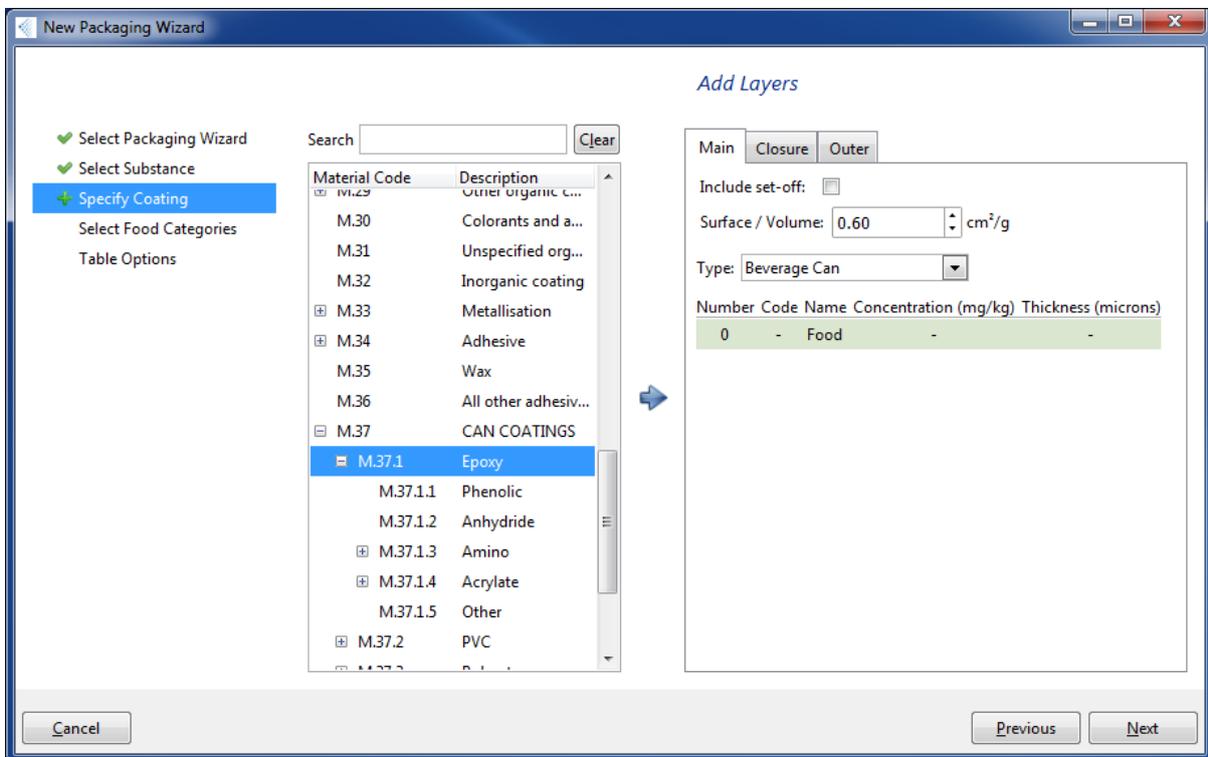


Figure 3-37: Accessing Full Material Code

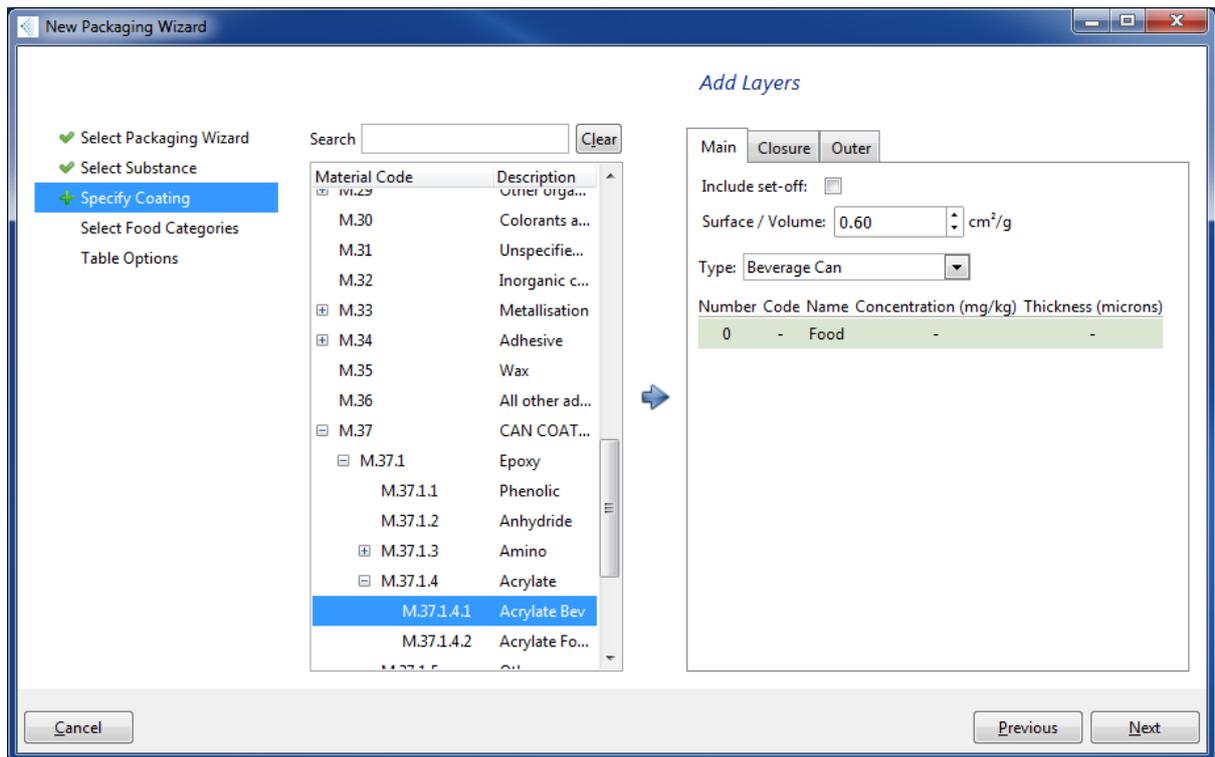


Figure 3-38: Viewing Full Material Code

Once the user has found the correct “Material Code”, and highlighted it (as in Figure 3-38), the next step is to click the blue arrow. This has the effect of displaying this material as illustrated in Figure 3-39.

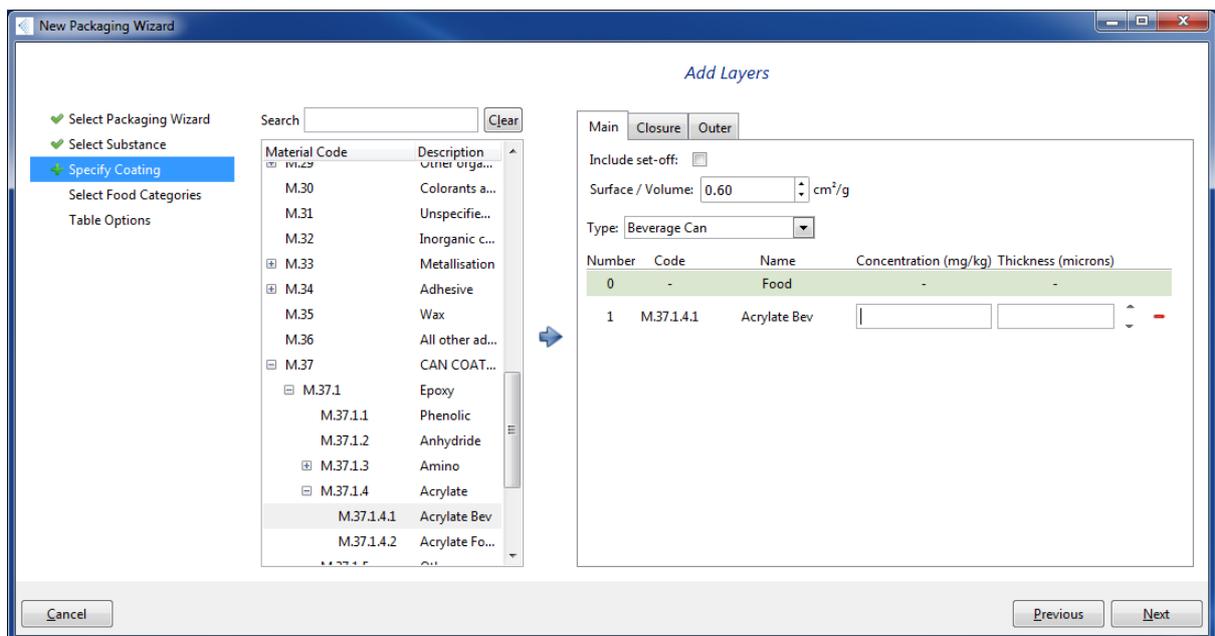


Figure 3-39: Selection of Material Code

The user is asked to enter the initial concentration of the chosen substance in the material as well as the thickness of the material. This step is illustrated in Figure 3-40.

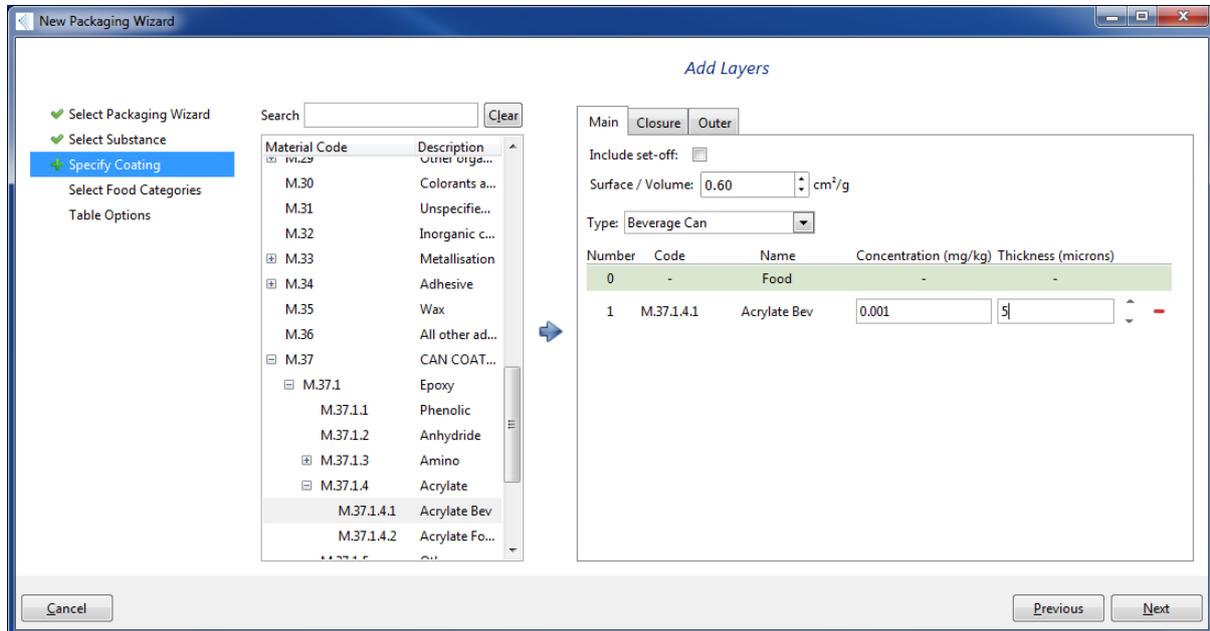


Figure 3-40: Filling in Concentration and Thickness values

Now the user selects the Food Categories of interest. In this example, Beer is selected as illustrated in Figure 3-41.

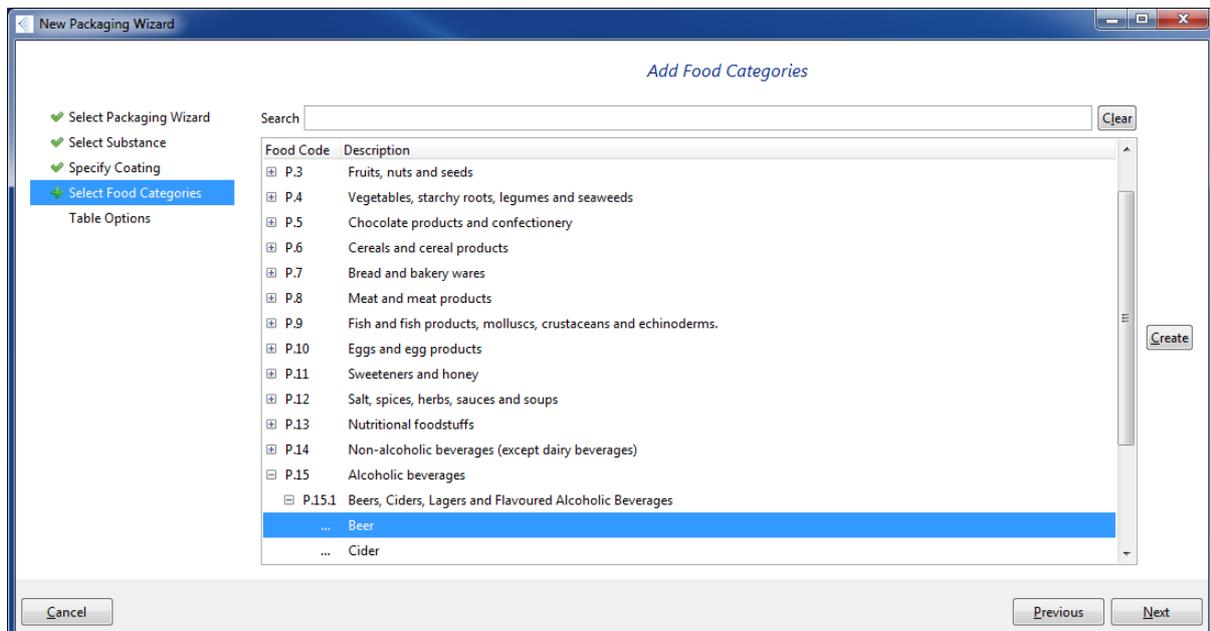


Figure 3-41: Selection of appropriate Food Categories

A “Pack Size” and “Substance Migration Rate” are required as part of the assessment. This is illustrated in Figure 3-42 and Figure 3-43.

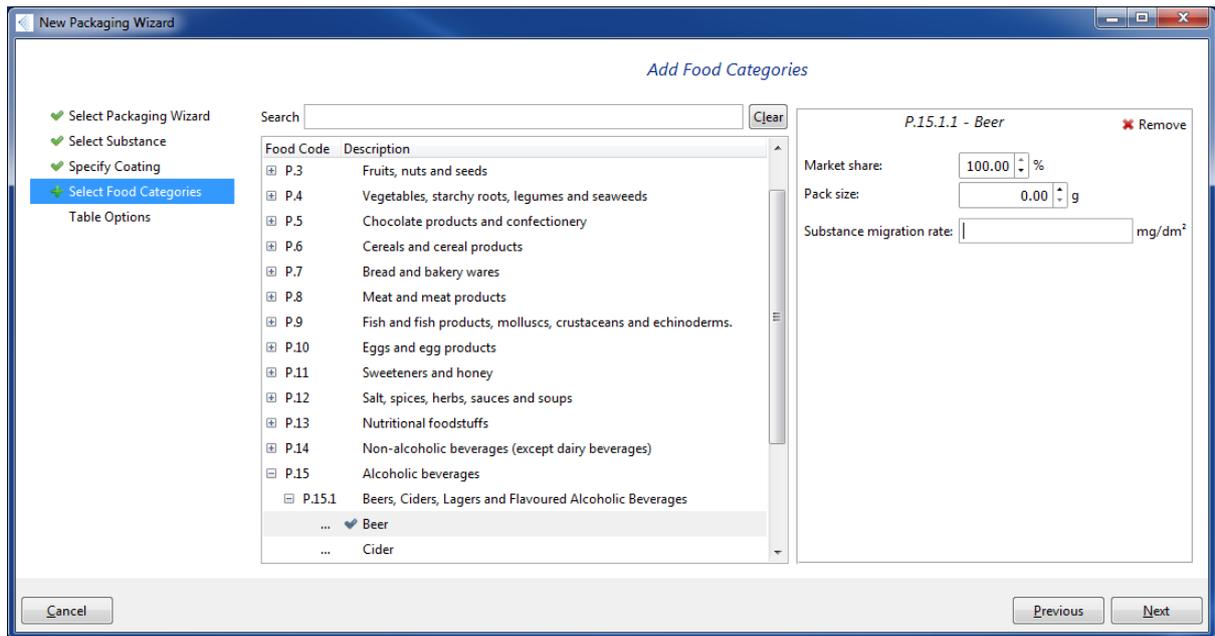


Figure 3-42: Pack Size and Migration Rate

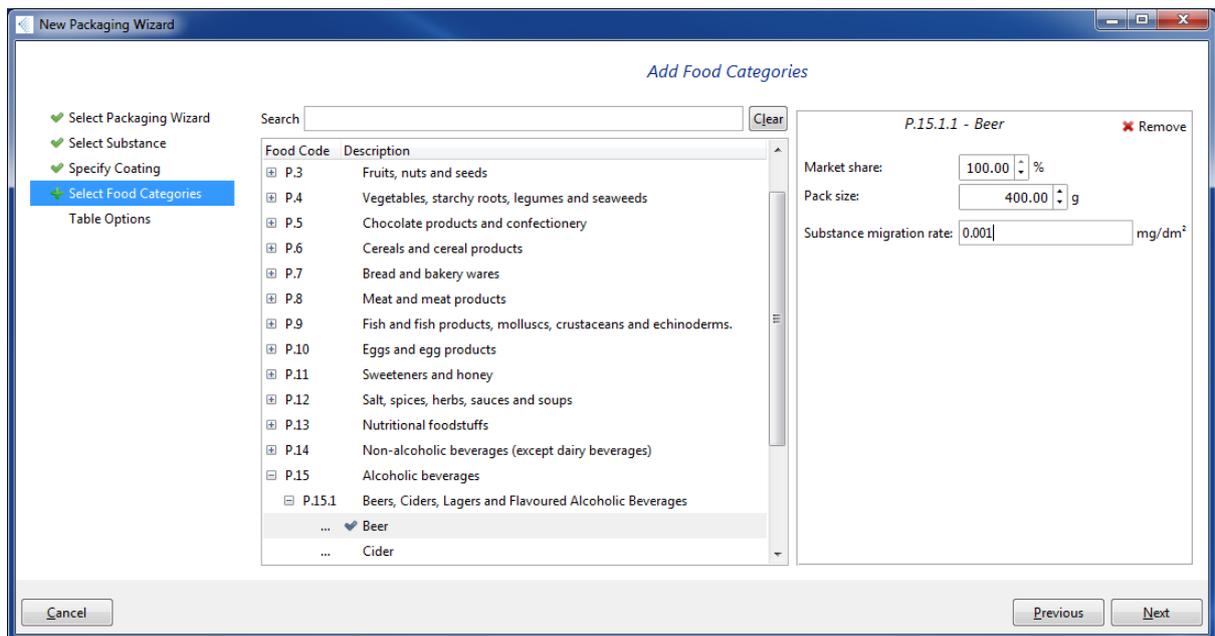


Figure 3-43: Entering Pack Size and Substance Migration Rate

As in other assessments, it is preferable to choose an appropriate name for the assessment. This step is illustrated in Figure 3-44 and Figure 3-45.

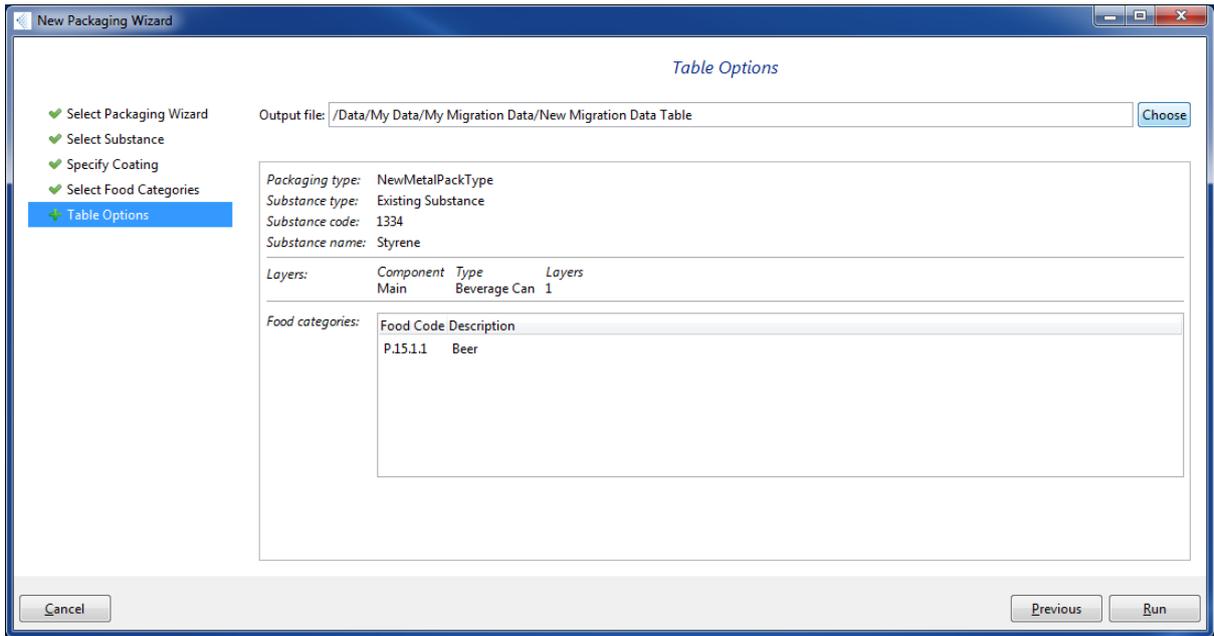


Figure 3-44: Name File

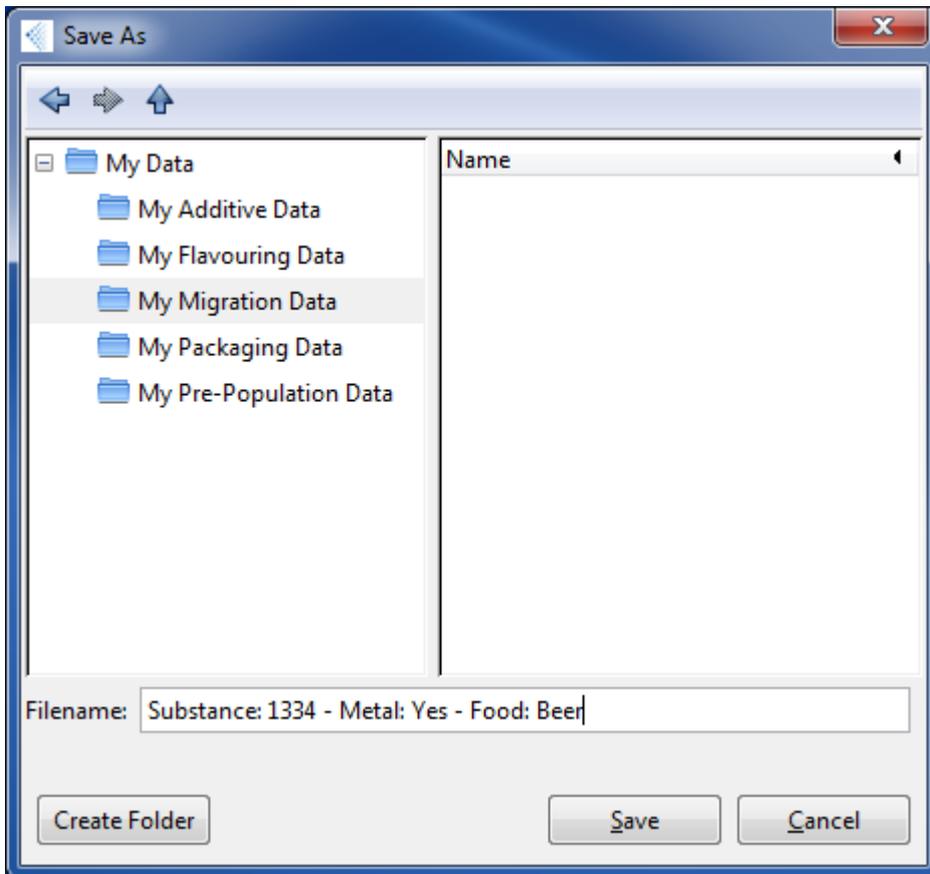
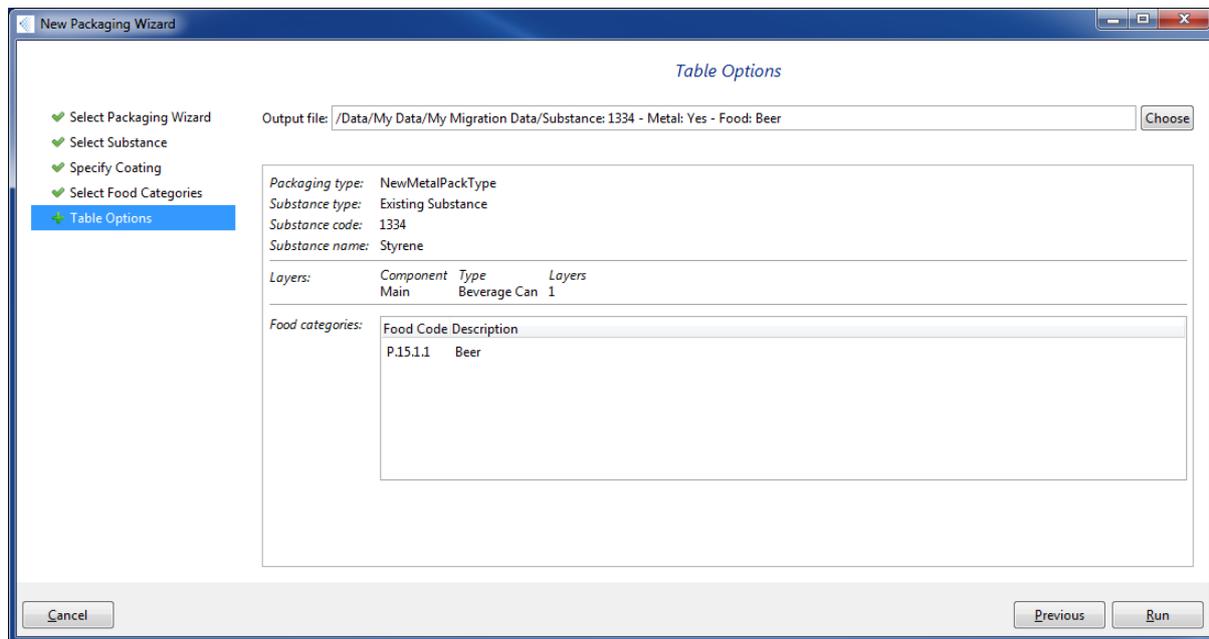


Figure 3-45: Naming File

A summary of the assessment is provided and the user selects “Run” to run the assessment. This is illustrated in Figure 3-46 and Figure 3-47.



Summary of Assessment

Figure 3-46: Summary of Assessment

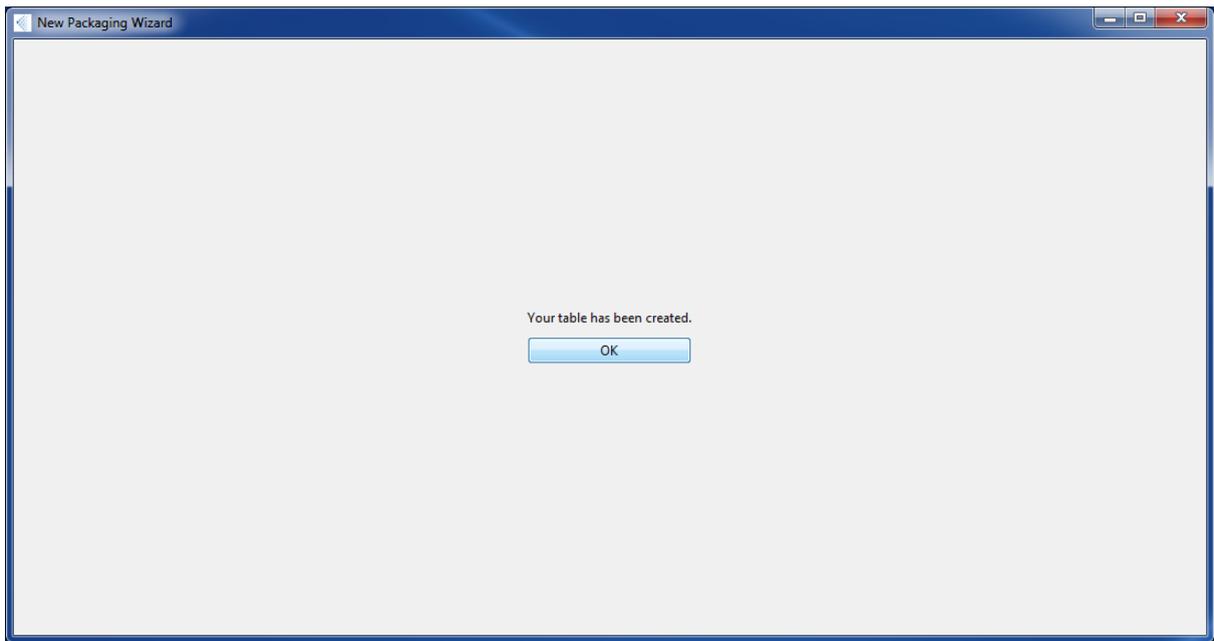


Figure 3-47: Table Created

Upon completion of the assessment, the software informs the user as shown in Figure 3-48.

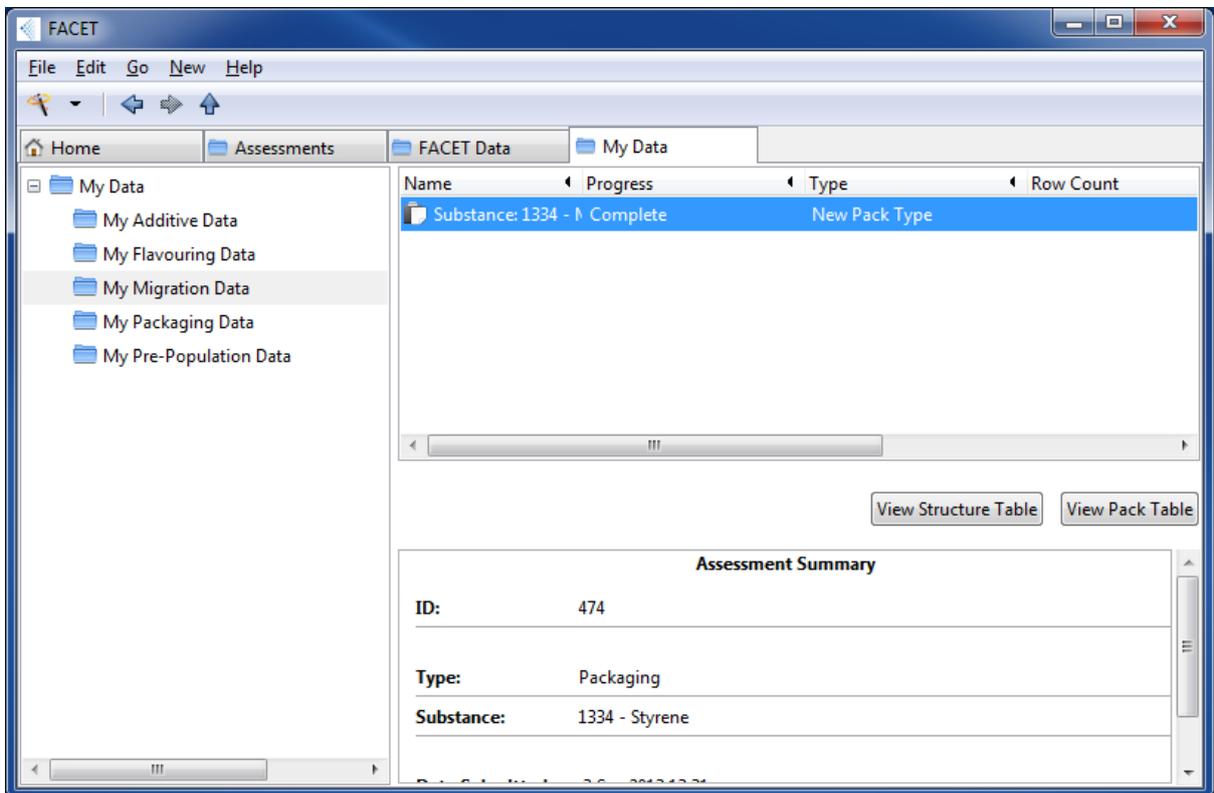


Figure 3-48: Assessment Complete

The full name of the table can be viewed by extending the “Name” field until the full name is visible. This is illustrated in Figure 3-49.

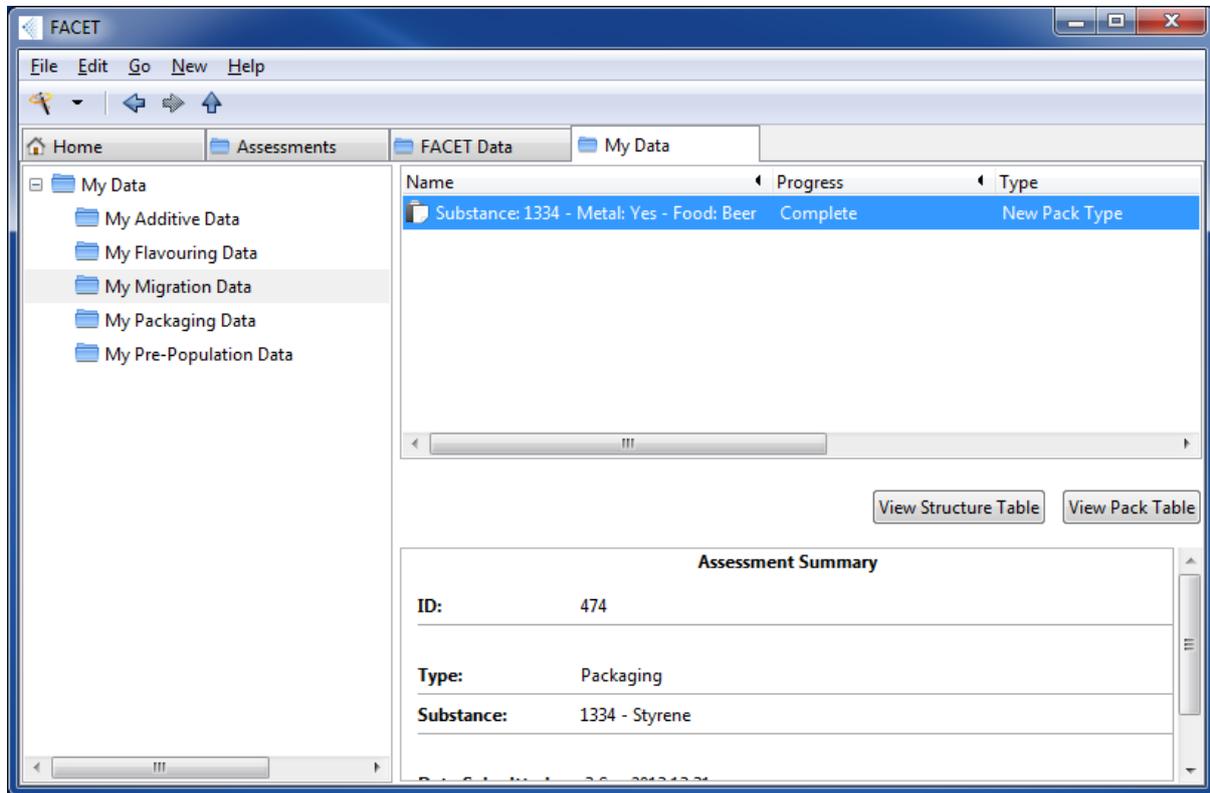


Figure 3-49: Viewing Full Table Name

The software does not allow the user to view the concentration data which is a result of the assessment. However, the concentration data is available to be used in a Packaging Assessment and is described visually in Figure 3-53 to Figure 3-70. It is possible however to view the “Structure Table” and “Pack Table” which are associated with the assessment above. This is possible by clicking the “View Structure Table” or “View Pack Table” options shown in Figure 3-50. Both options are illustrated in Figure 3-51 and Figure 3-52 respectively.





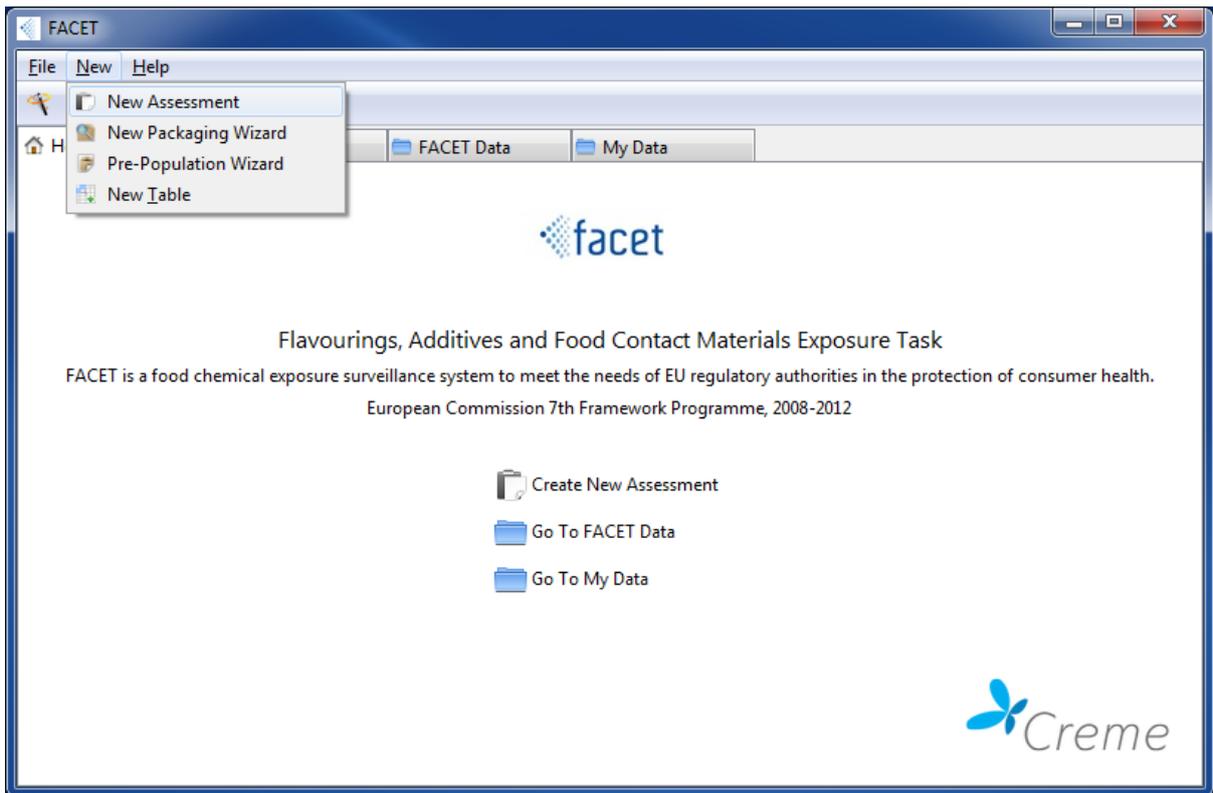


Figure 3-53: Running New Assessment

Next, the user selects “Packaging Assessment” as shown in Figure 3-54.

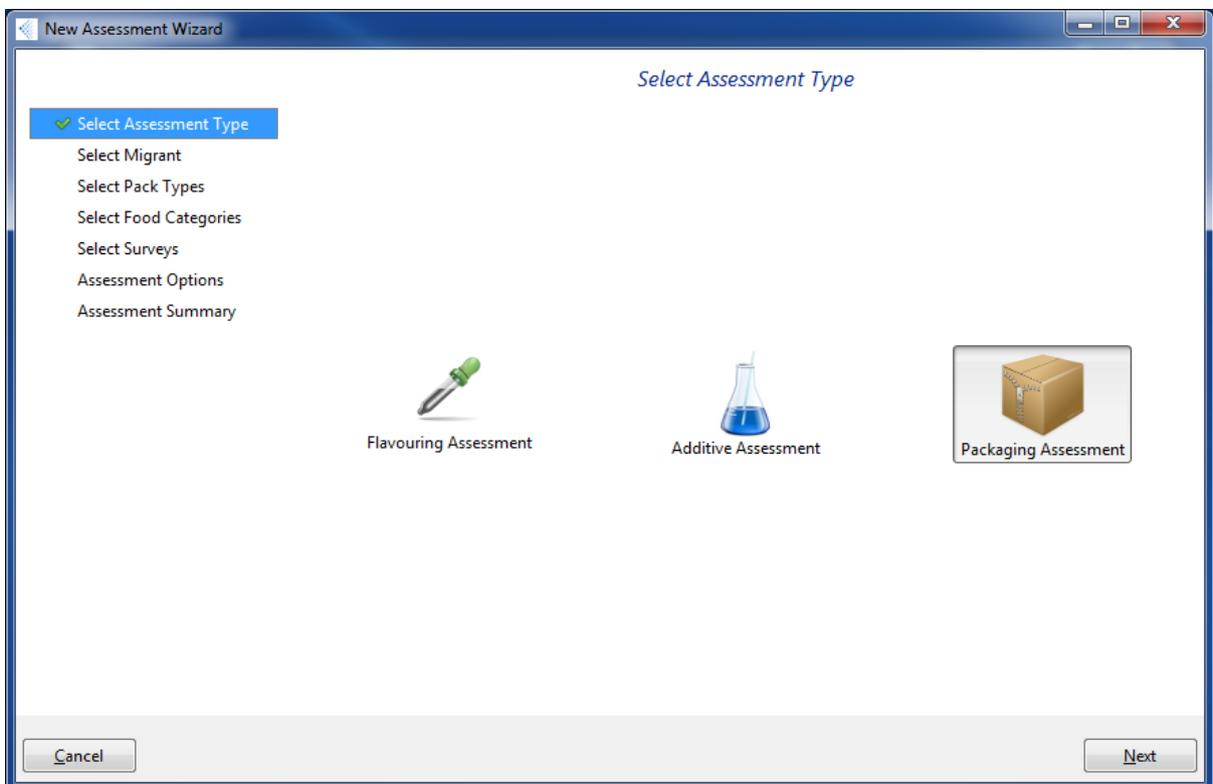


Figure 3-54: Select Packaging Assessment

At the next step, the user selects “My Concentration Data” as illustrated in Figure 3-55.

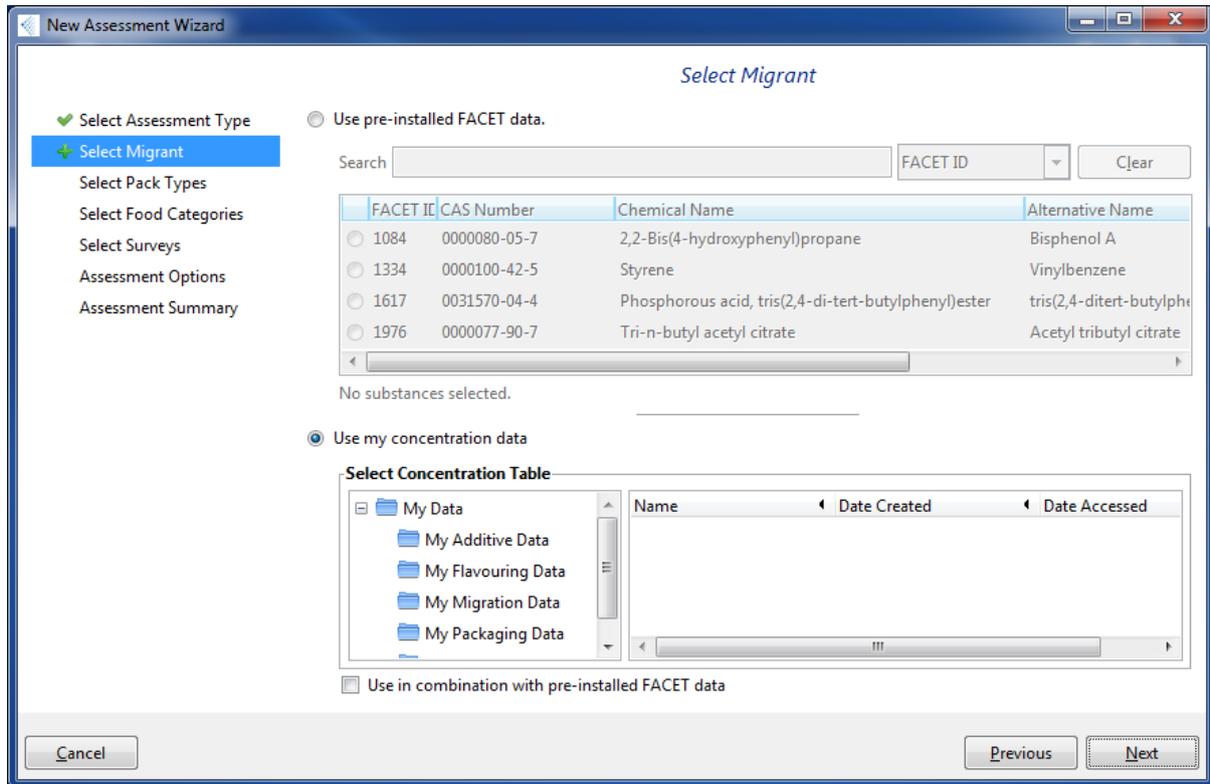


Figure 3-55: Use my concentration data

The table of interest is “Substance: 1334 – Metal: Yes – Food: Beer”. This is located in the “My Migration Data” folder as shown in Figure 3-56 and Figure 3-57.

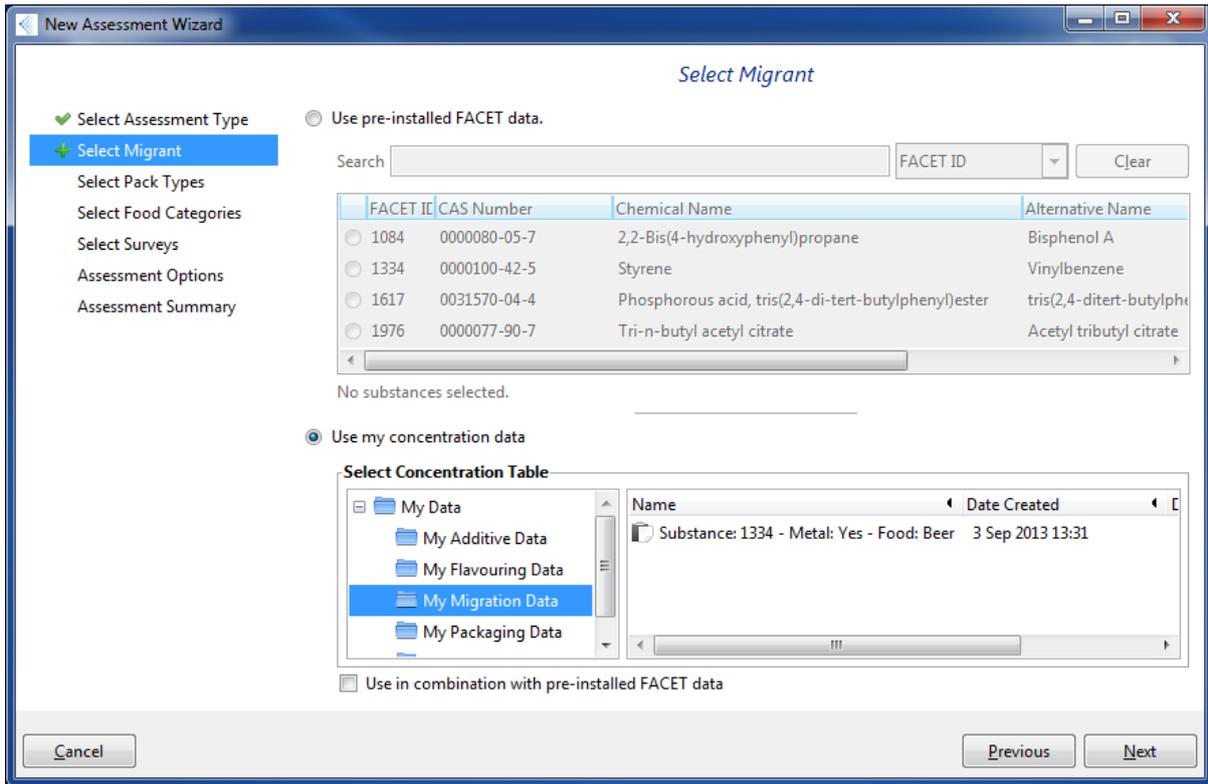


Figure 3-56: Selection of Appropriate Folder

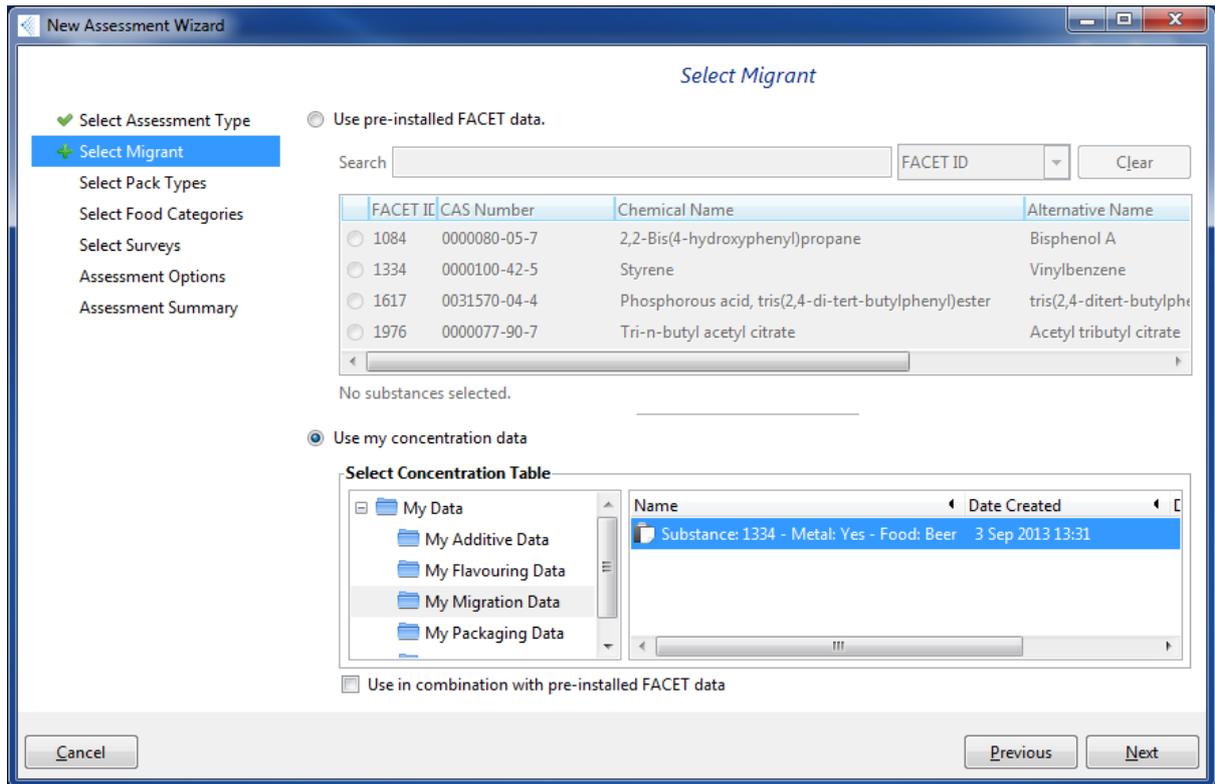


Figure 3-57: Selection of Appropriate Table

At this stage, the user selects the pack types and food categories that are of interest. In this example, we consider “All” pack types and the food category “P.15.1.1 Beer”. This is shown in Figure 3-58 and Figure 3-59.

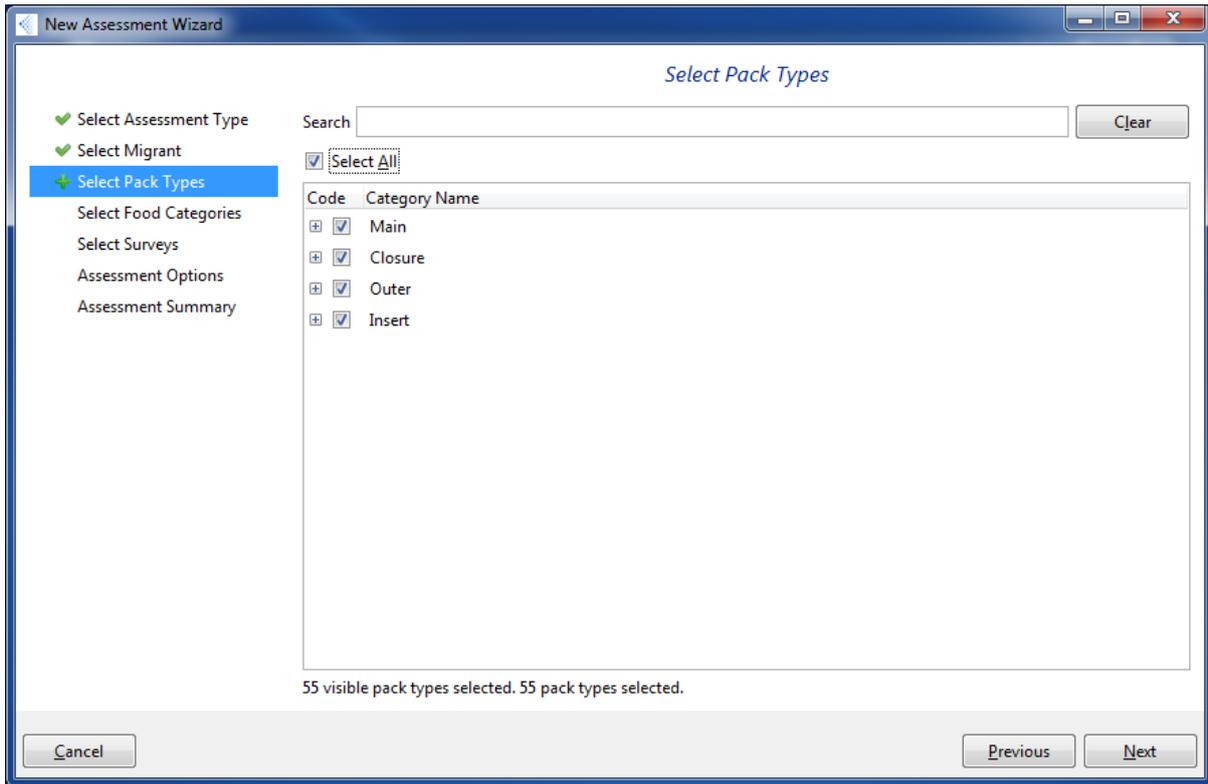


Figure 3-58: Select Pack Types

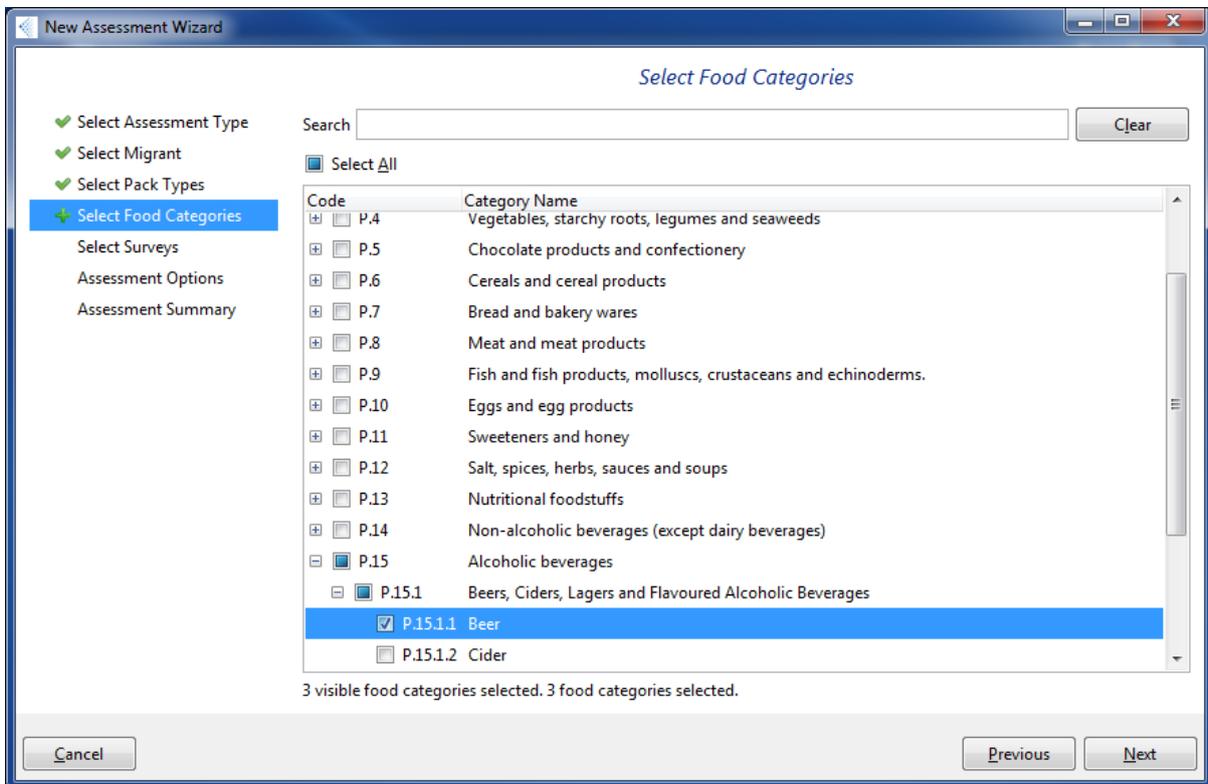


Figure 3-59: Select Food Categories

The appropriate survey is chosen (as shown in Figure 3-60).

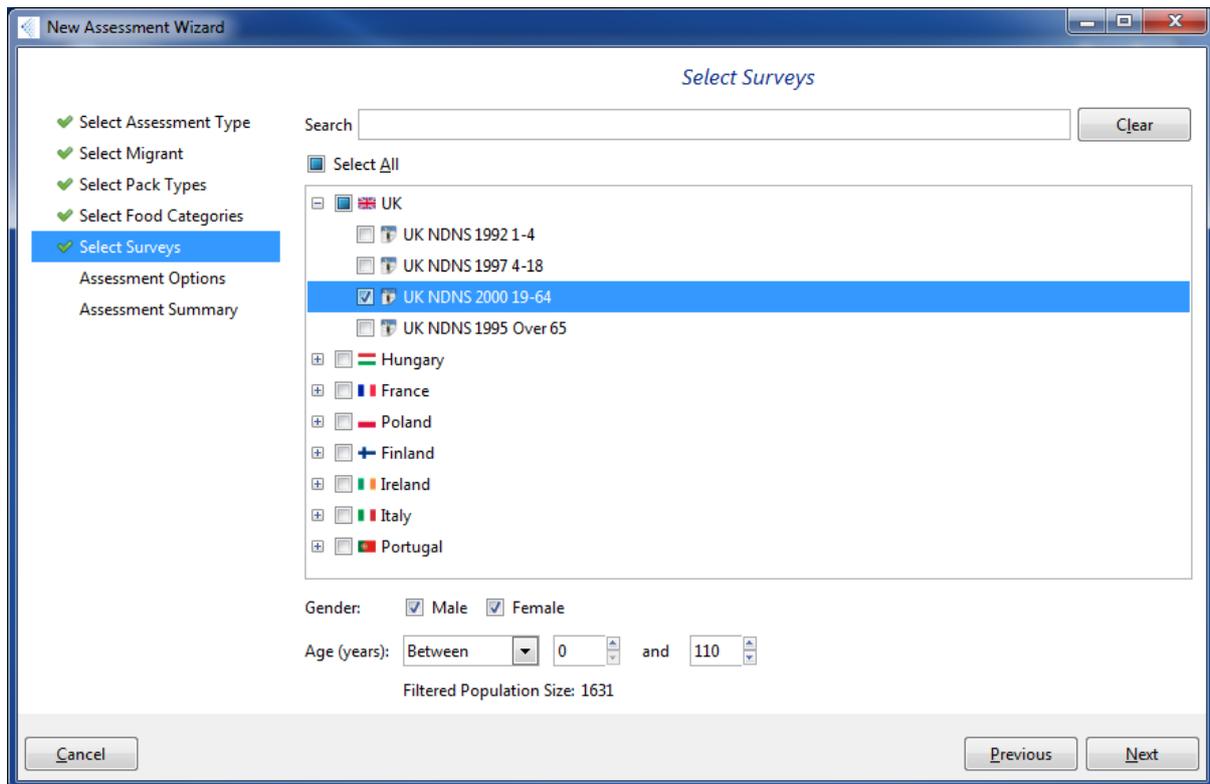


Figure 3-60: Select Survey

The user then has the opportunity to select various Assessment Options. This step is illustrated in Figure 3-61 to Figure 3-63.

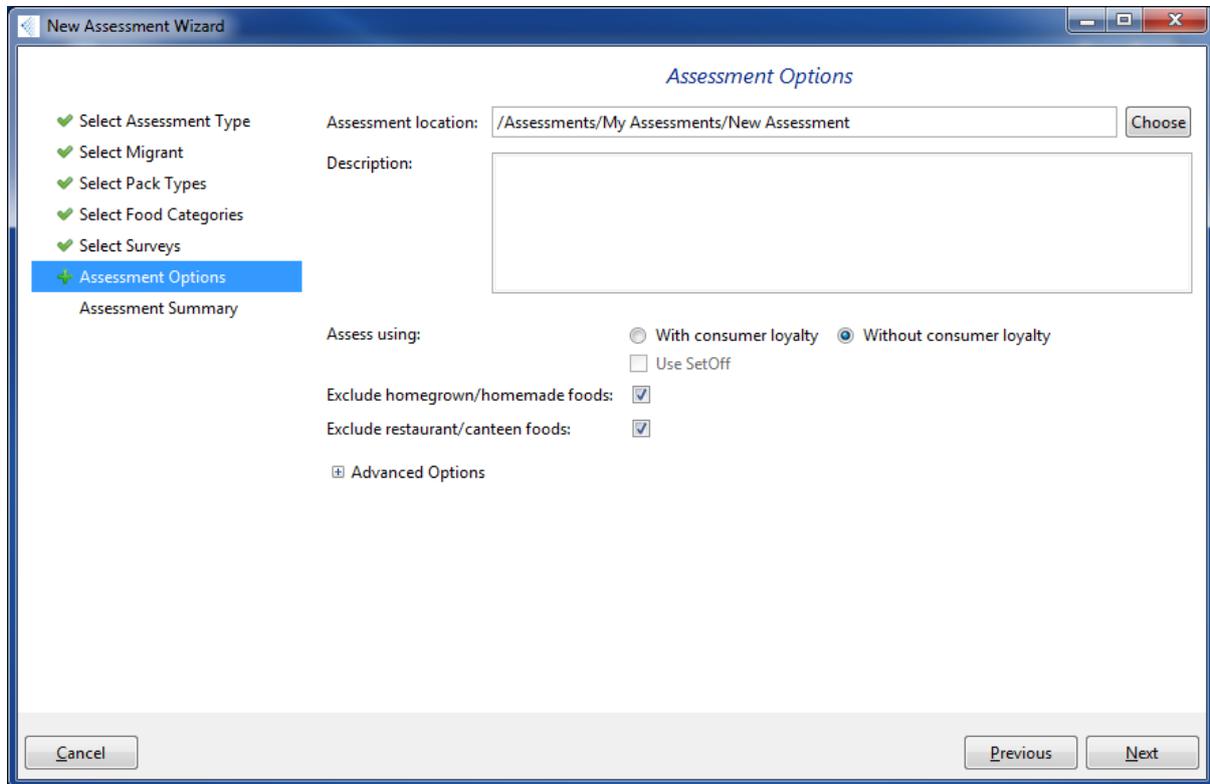


Figure 3-61: Assessment Options

In the advanced options, the user can select to “Include lower tier results” as well as adding to the default list of percentiles used. For our example, we leave the “Include lower tier results” box unticked and deselect the P25 percentile.

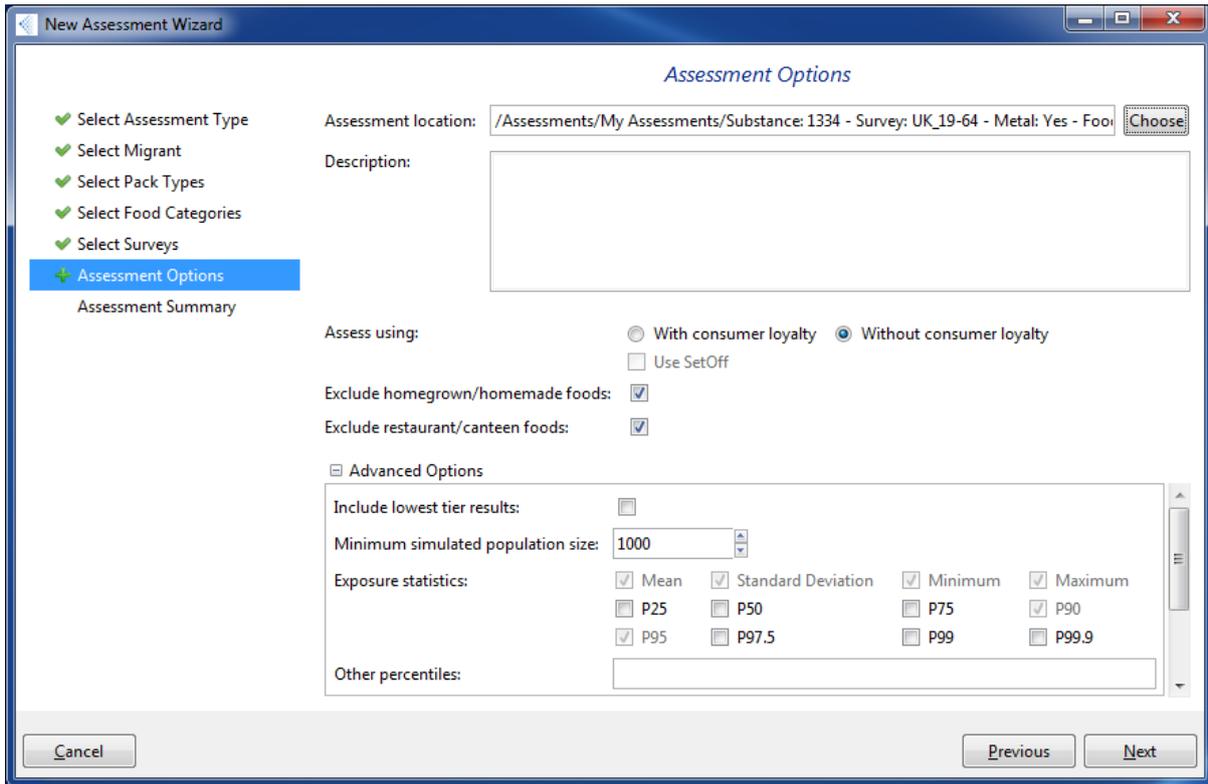


Figure 3-62: Name Assessment

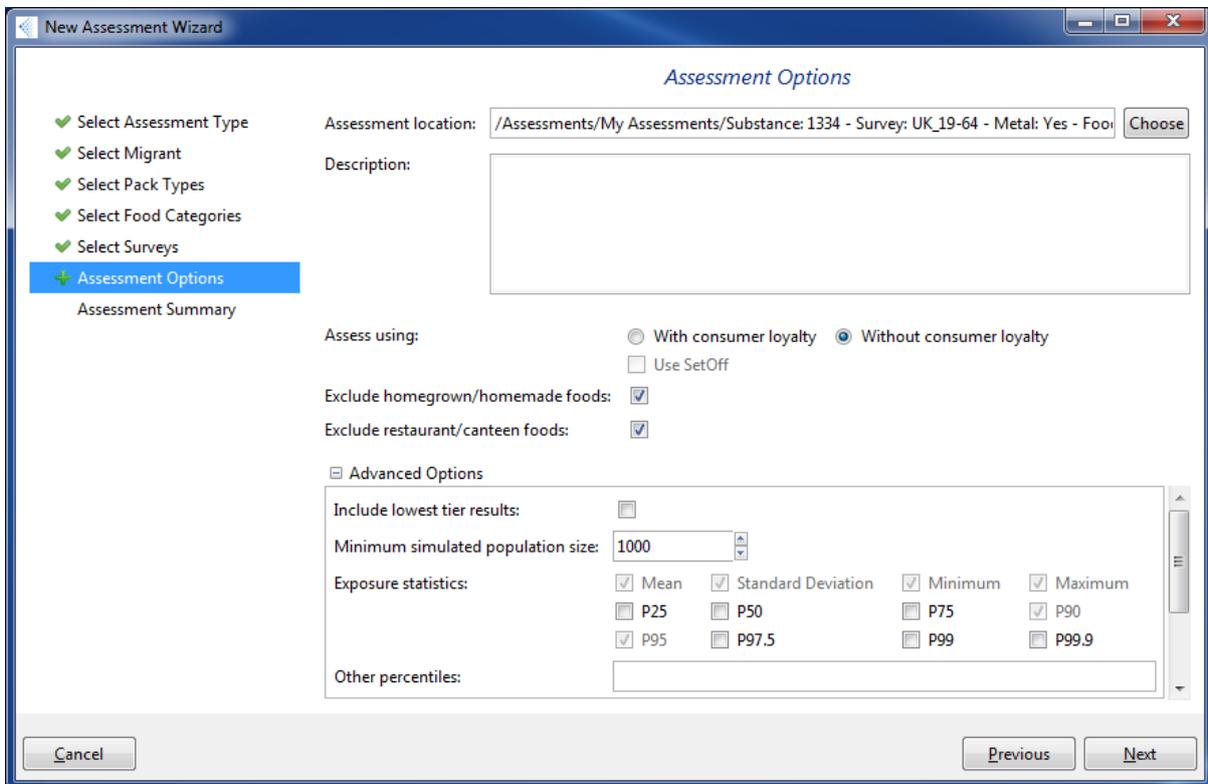


Figure 3-63: Advanced Options

At this stage, the Assessment is summarised and ready to be Run. This is illustrated in Figure 3-64 and Figure 3-65.

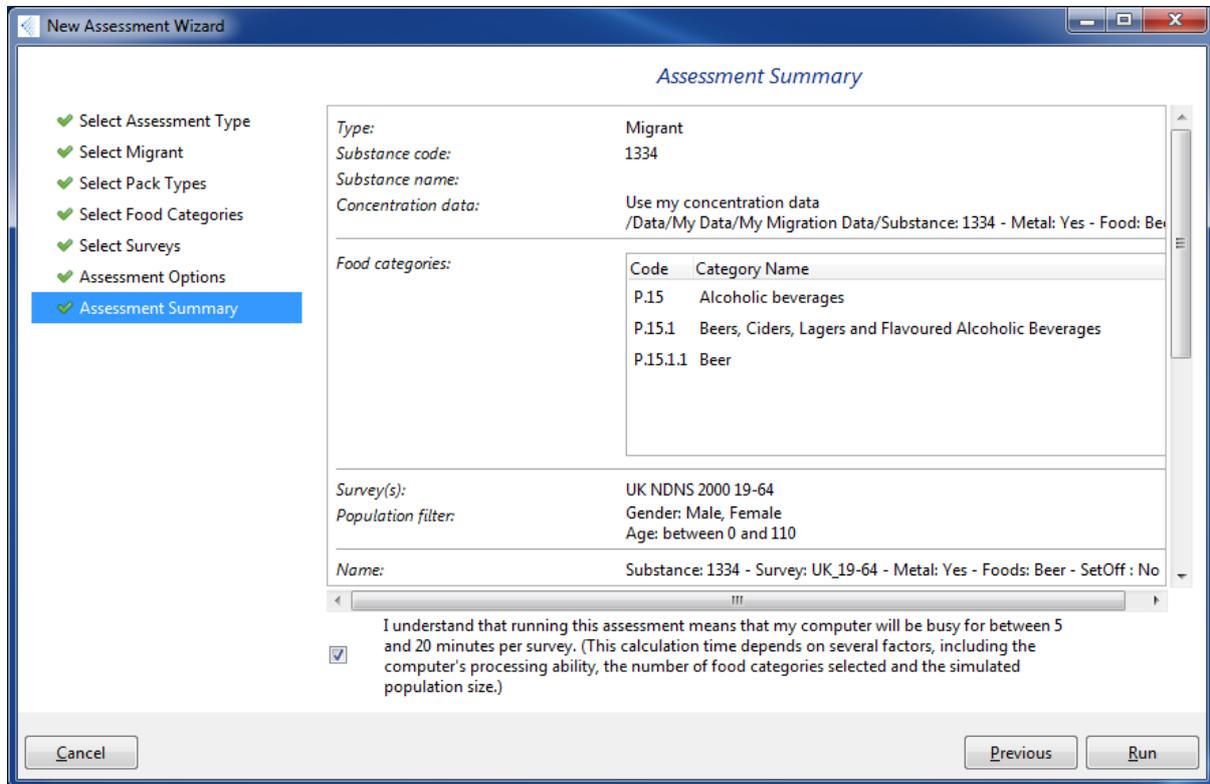


Figure 3-64: Assessment Summary

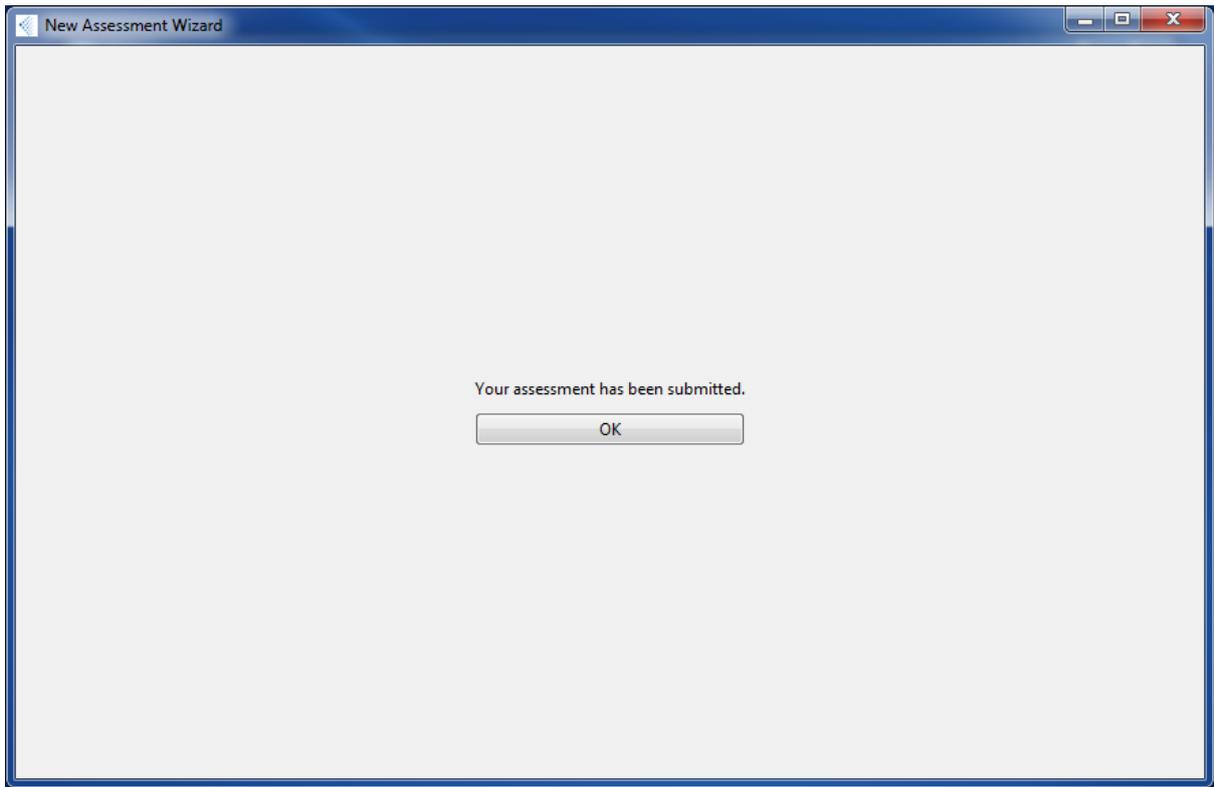


Figure 3-65: Assessment Submission Confirmation

Once the assessment is submitted, it begins by “Initialising” before moving into the “Progress” stage. At the end, the user is informed that the assessment has completed (i.e. “Complete”). This is illustrated in Figure 3-66 to Figure 3-68.

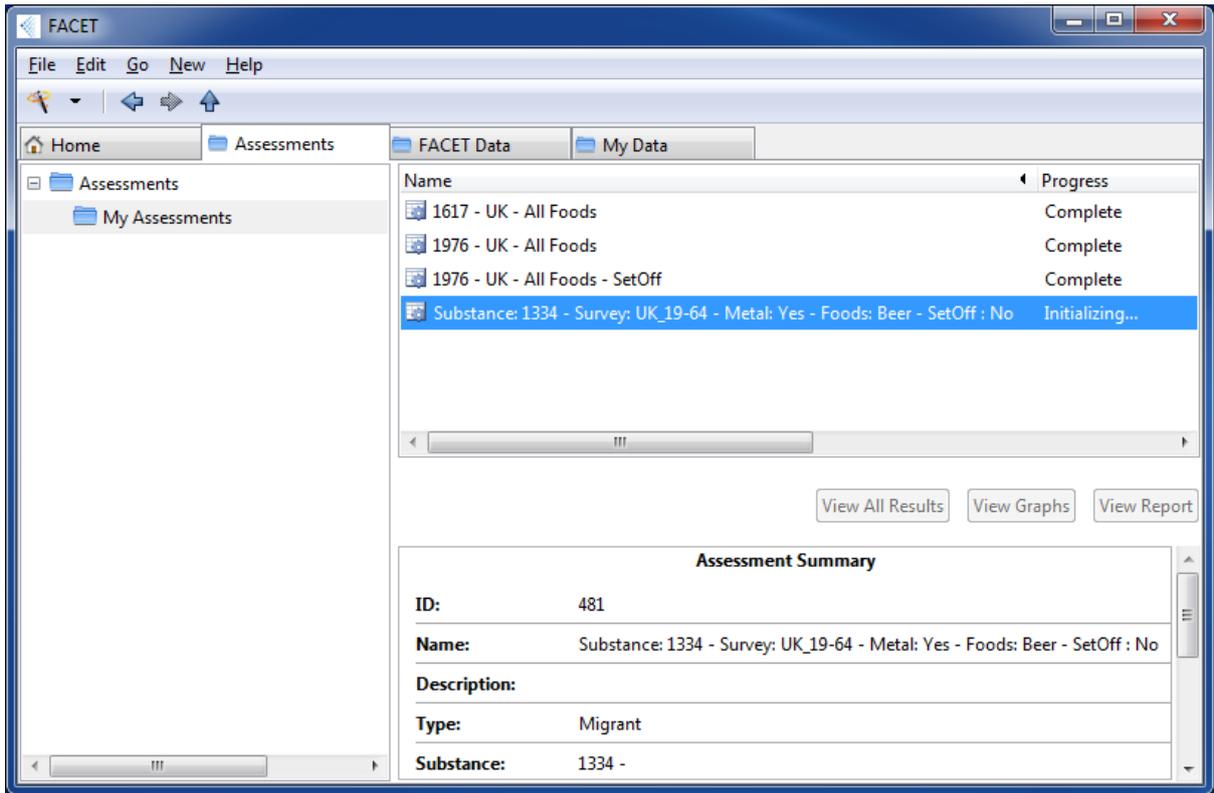


Figure 3-66: Assessment Initialising

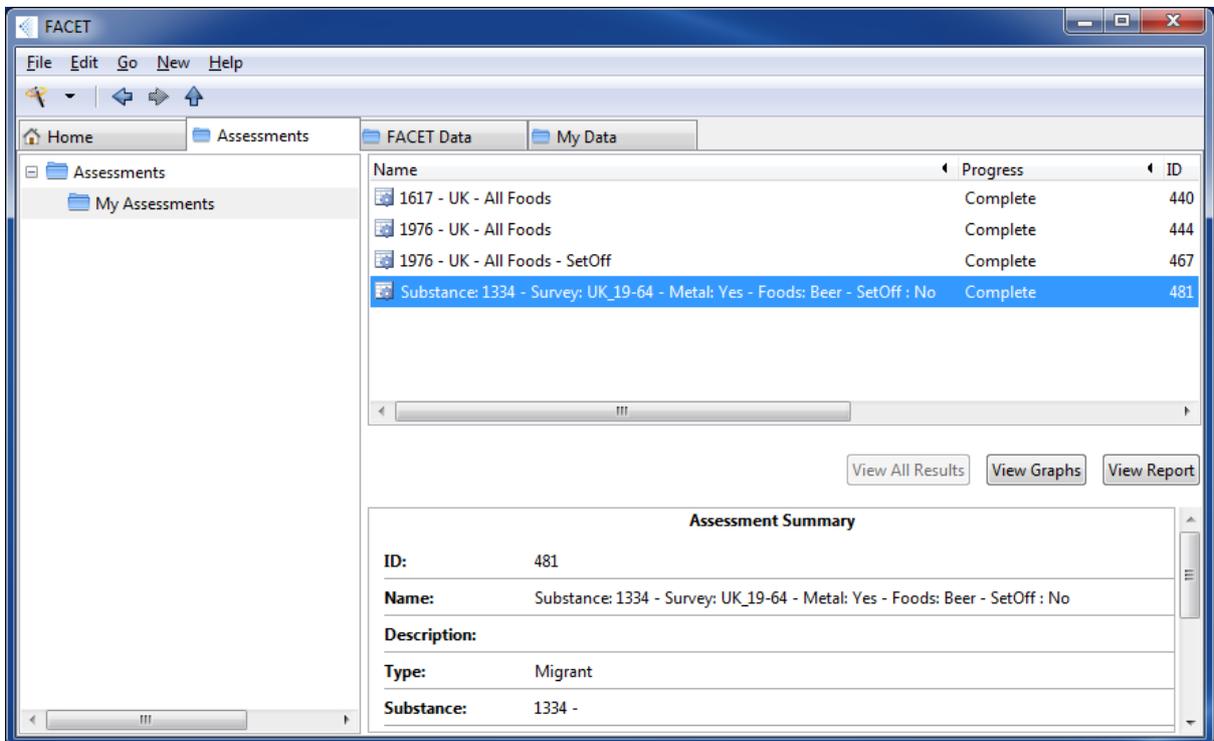


Figure 3-67: Assessment Complete

Following completion, the user has the option to view the results of the assessment. A similar approach to viewing the data is taken as in earlier parts of the manual. This is illustrated in Figure 3-68 to Figure 3-70.

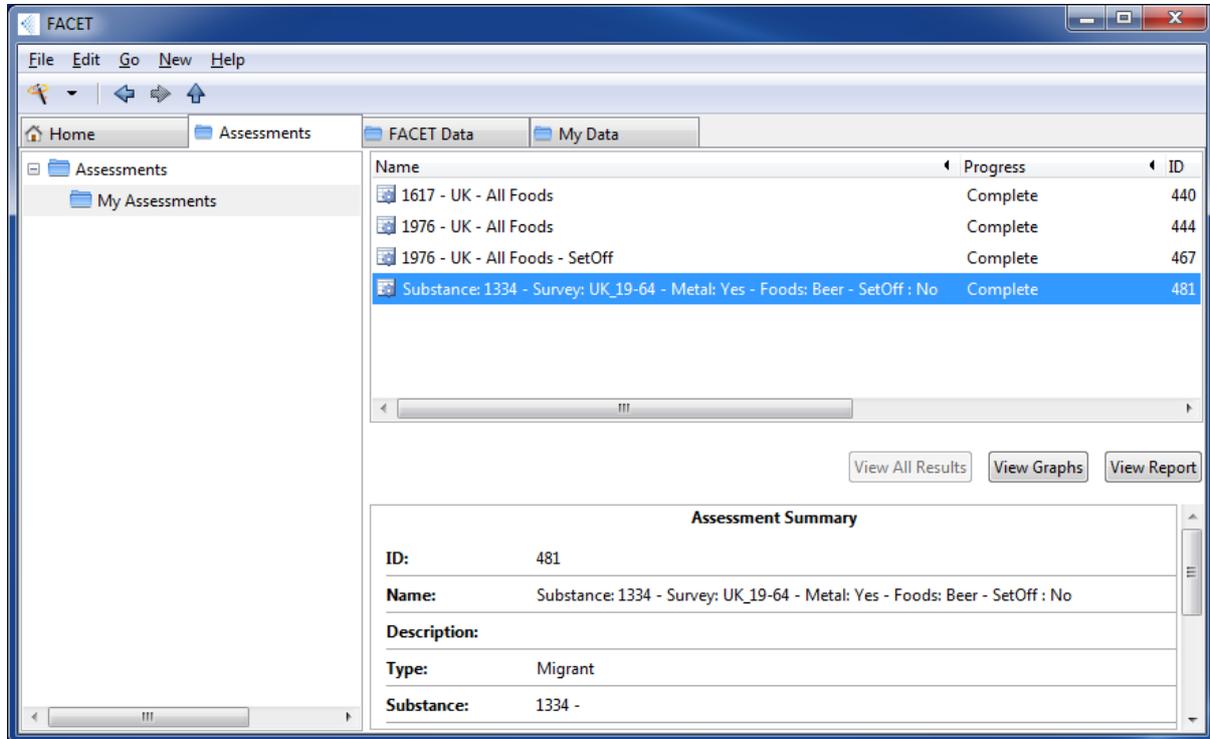


Figure 3-68: View Graphs

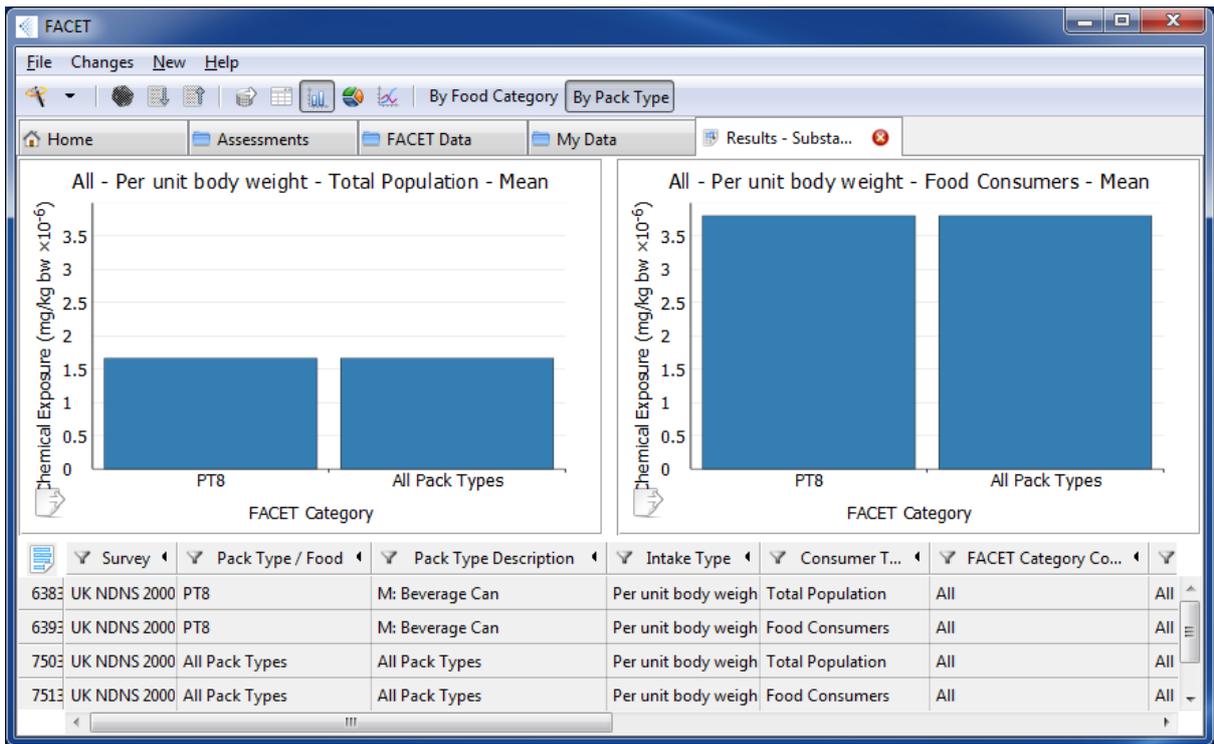


Figure 3-69: Graphs, by Pack Type

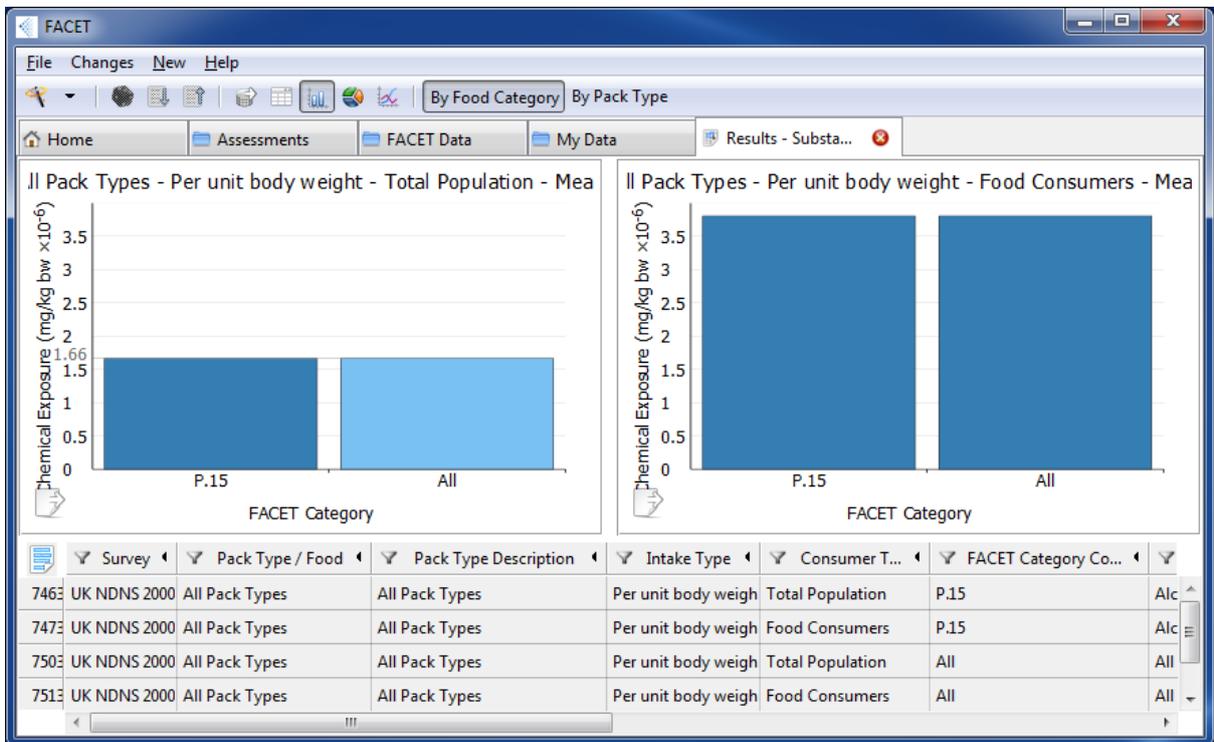


Figure 3-70: Graphs by Food Category

### 3.3.2 Using the New Packaging Wizard for a Substance in a Non-Metal Pack Type

As in the case of a substance in a metal pack, described in Section 3.3.1, a similar approach can be taken for substance in non-metal pack types. We consider the substance styrene (Facet Id = 1334) in this example. The earlier steps in the assessment are illustrated in Figure 3-71 to Figure 3-76.

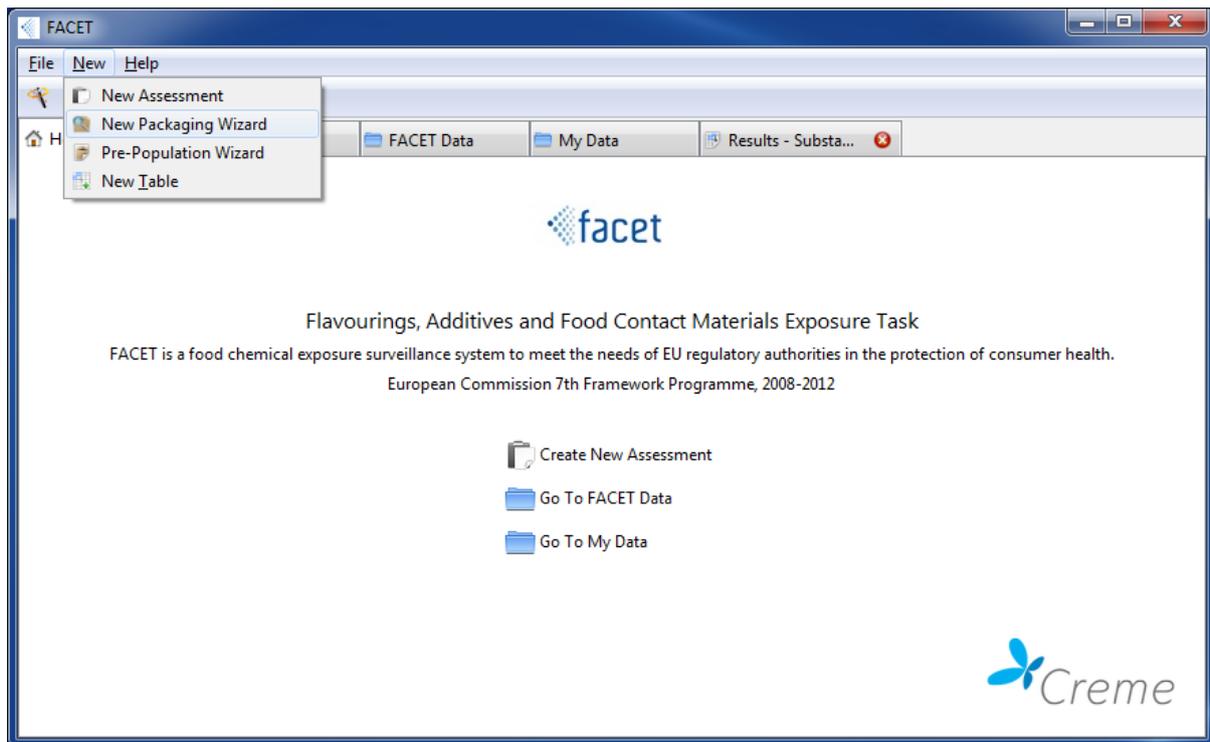


Figure 3-71: Select New Packaging Wizard

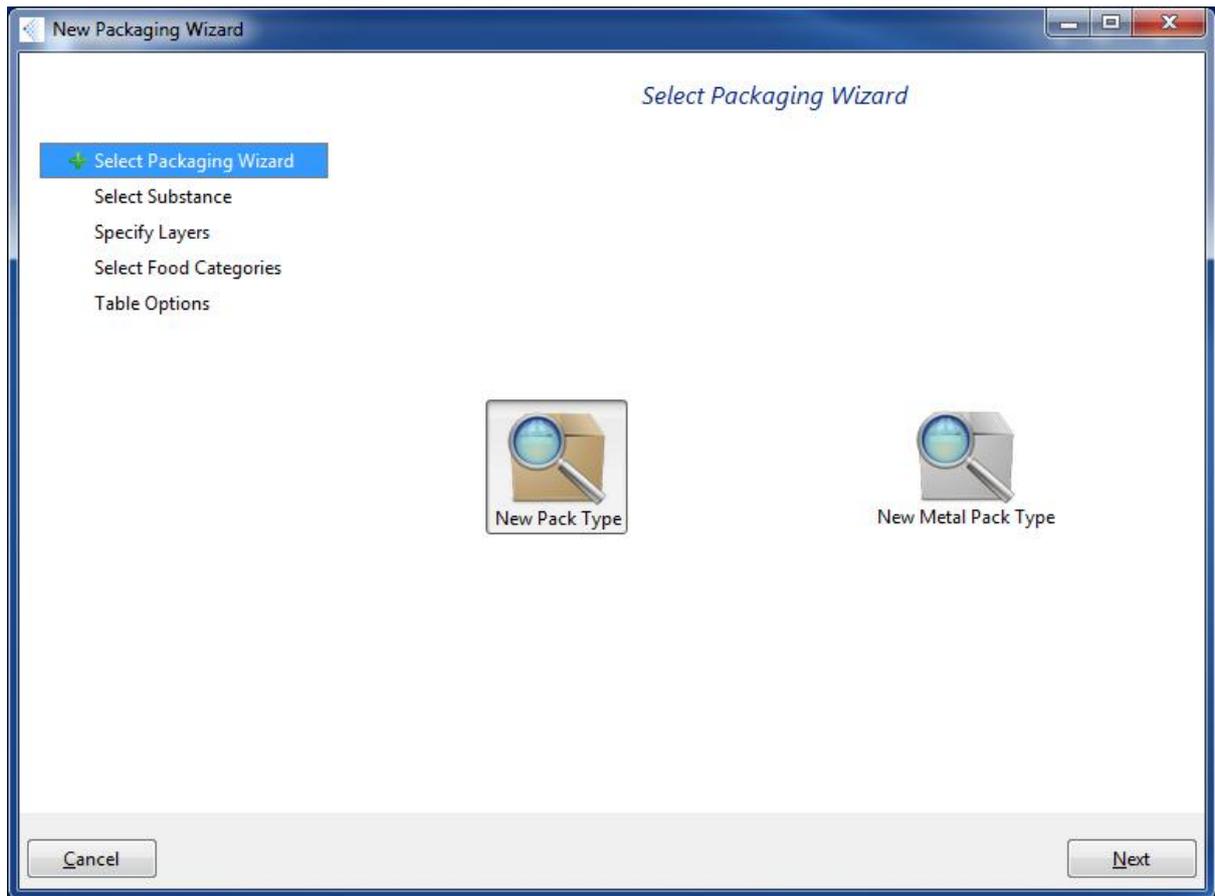


Figure 3-72: Select New Pack Type

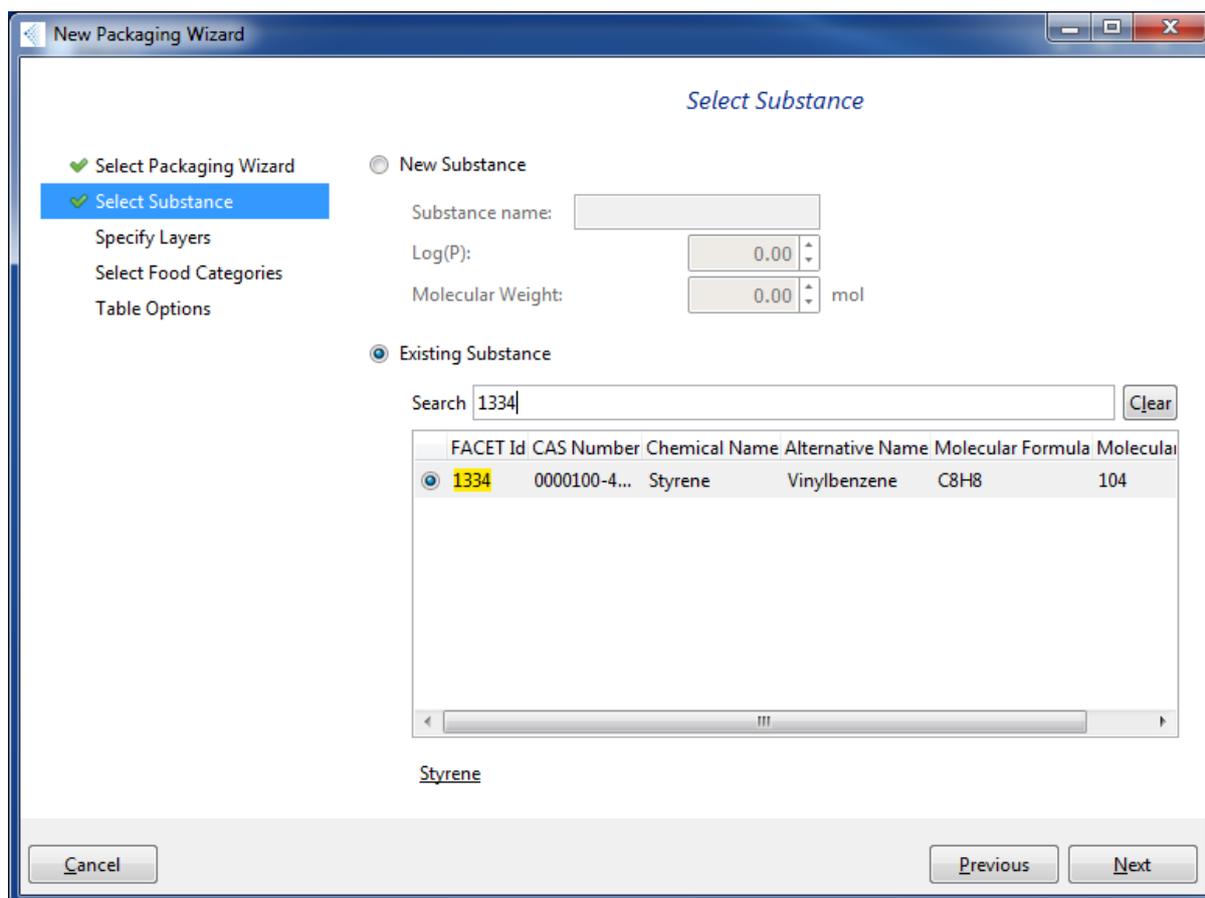


Figure 3-73: Select Substance

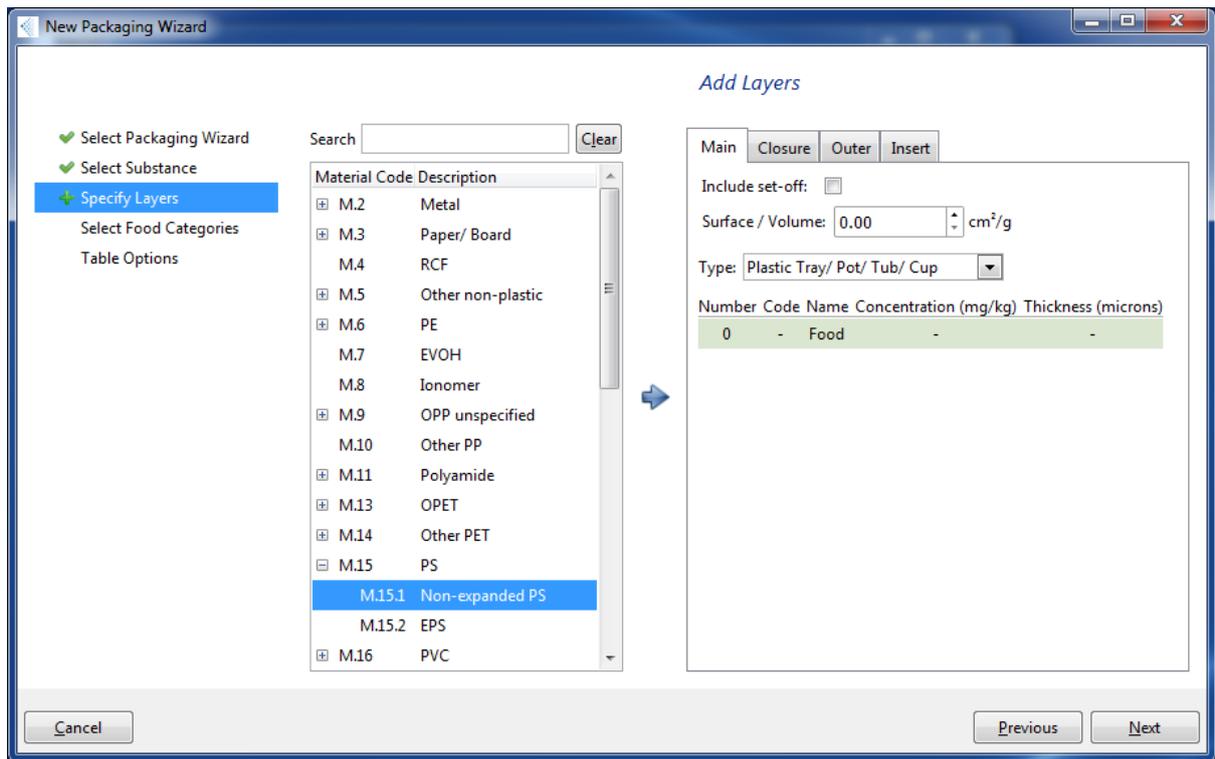


Figure 3-74: Select S/V ratio and Material Code

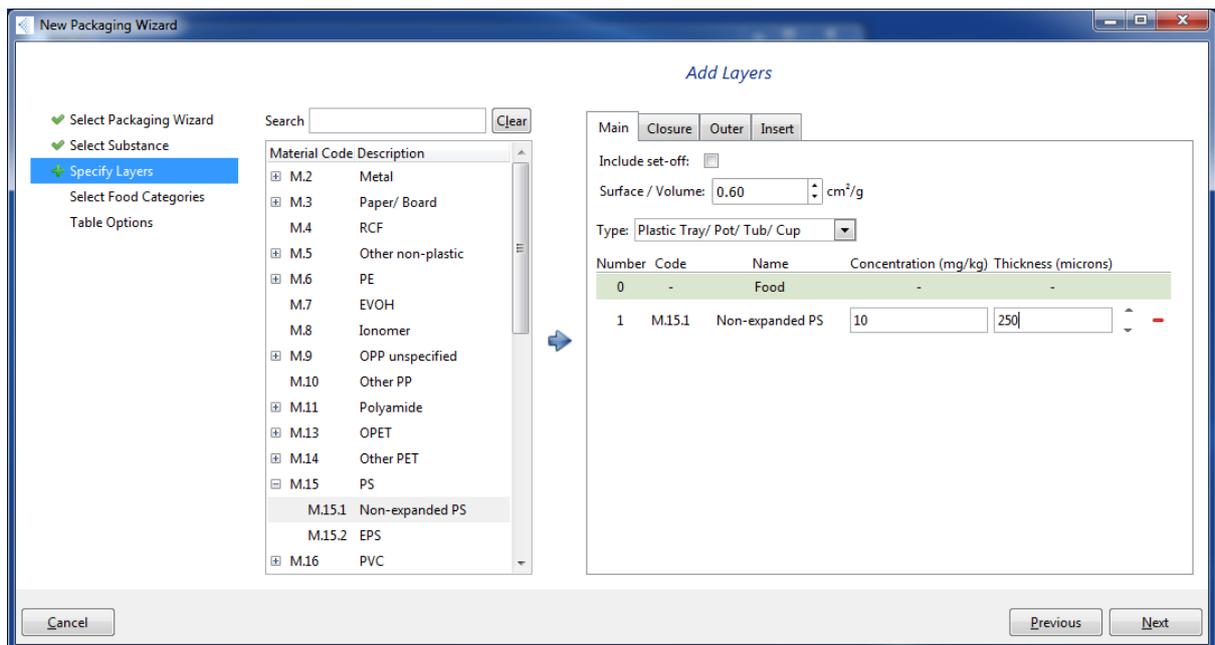


Figure 3-75: Select Concentration and Thickness

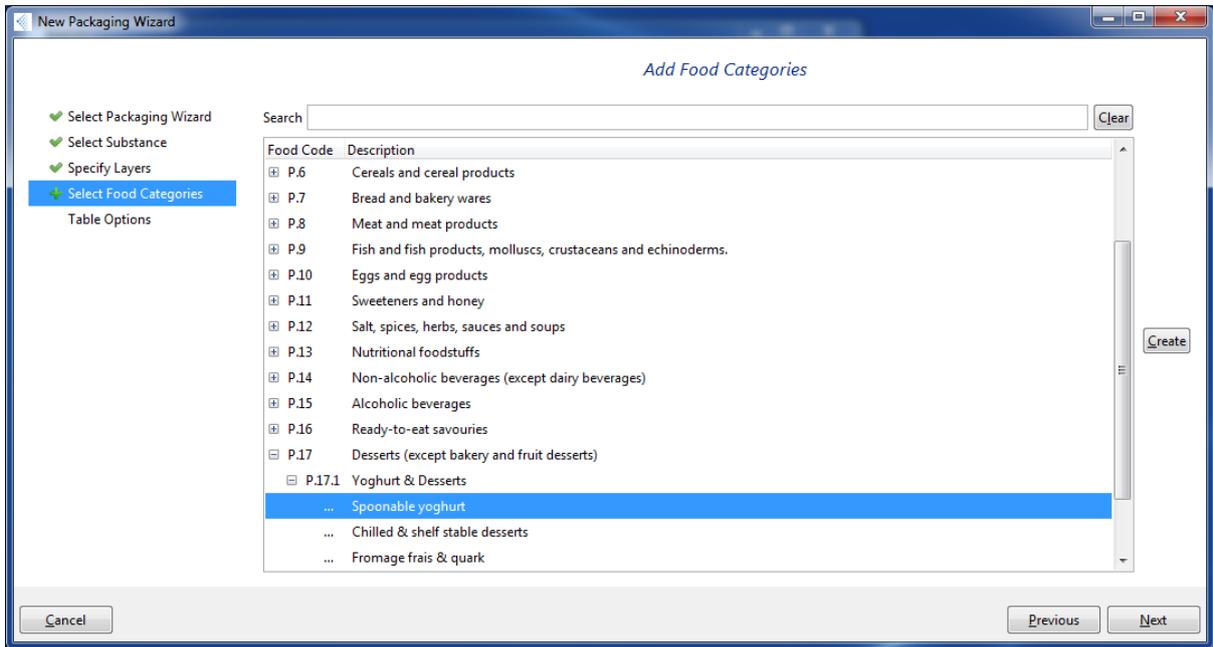


Figure 3-76: Select Food Categories

Once the Pack Types and Food Categories have been selected, the user needs to select the “Pack size” as well as the Time and Temperature regimes of interest. This is shown in Figure 3-77.

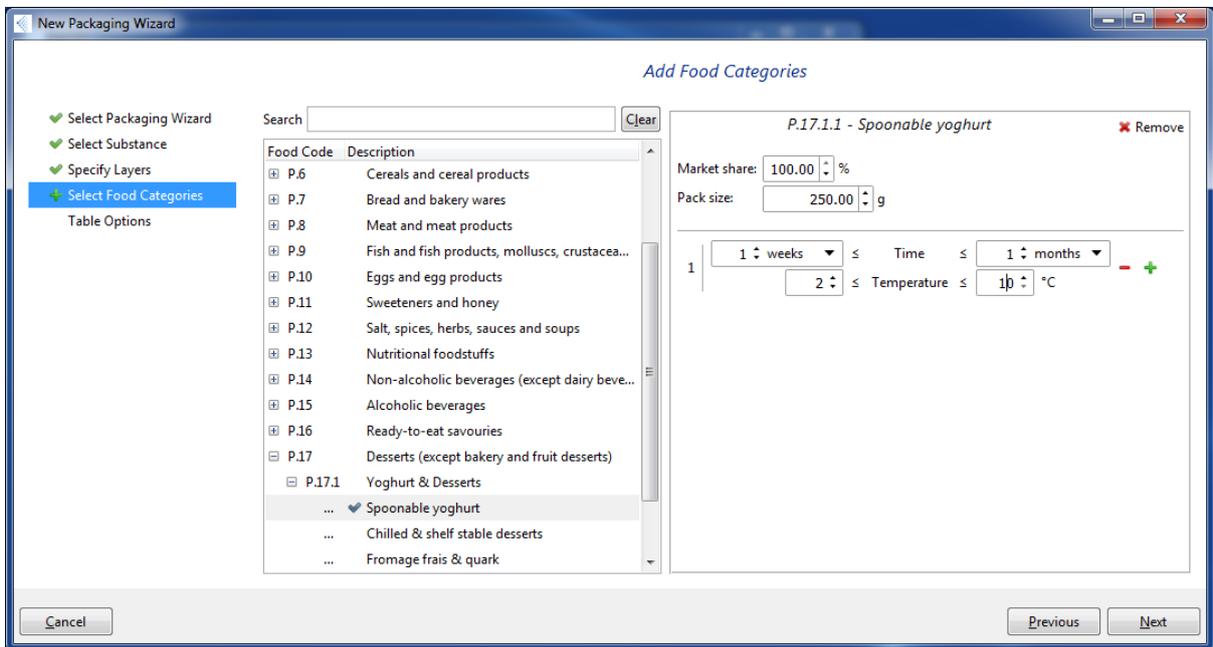


Figure 3-77: Selecting Time/temperature Regimes

The assessment is now ready to run. Before that a Table Name is given to the assessment as a reference to the details of the assessment and for easier access later. This is shown in Figure 3-78 and Figure 3-79.

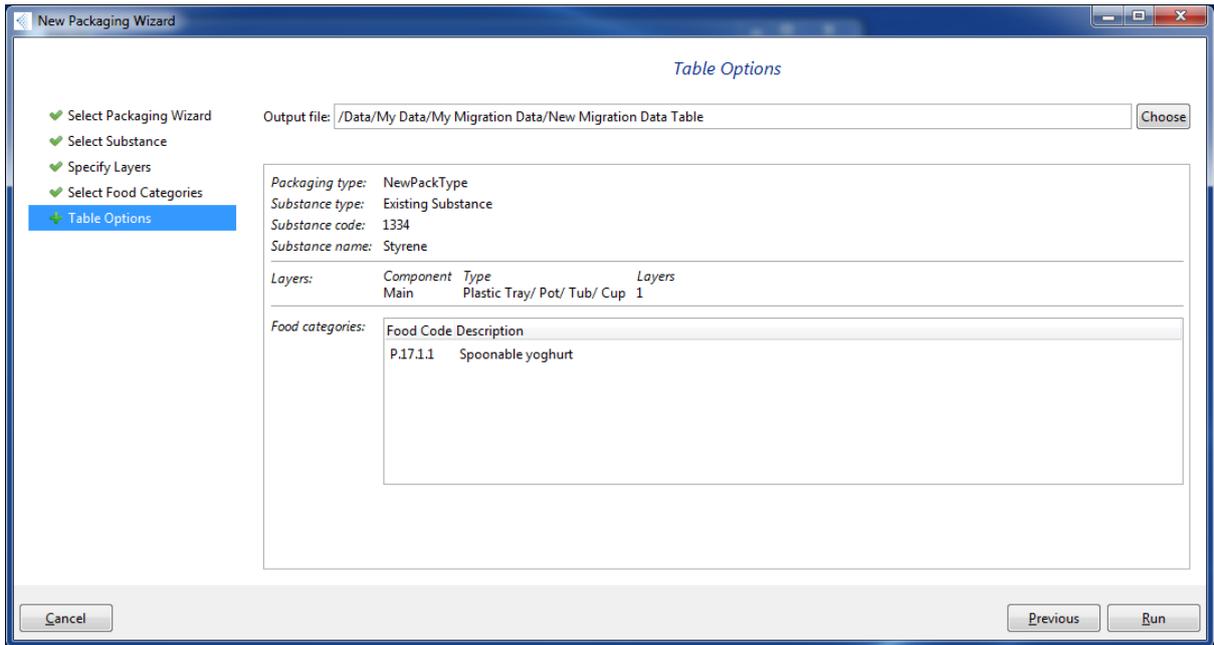


Figure 3-78: Table Options

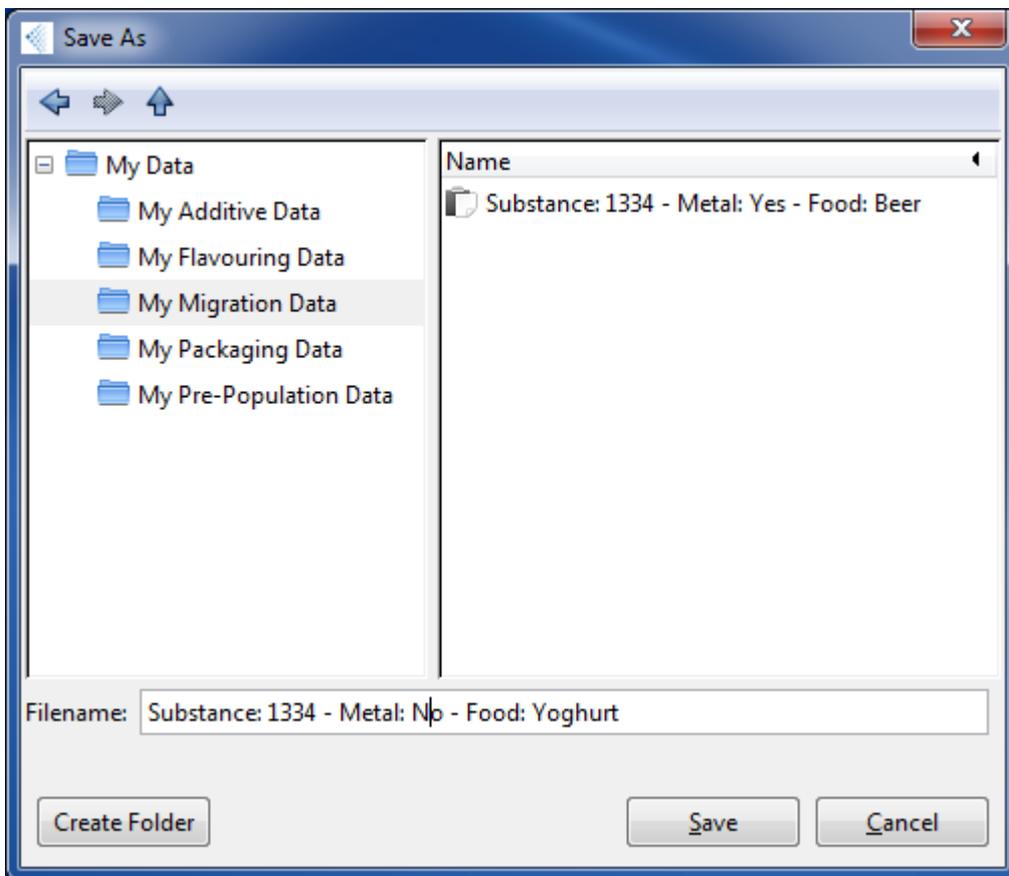


Figure 3-79: Naming Assessment

Now the assessment can be run as shown in Figure 3-80.

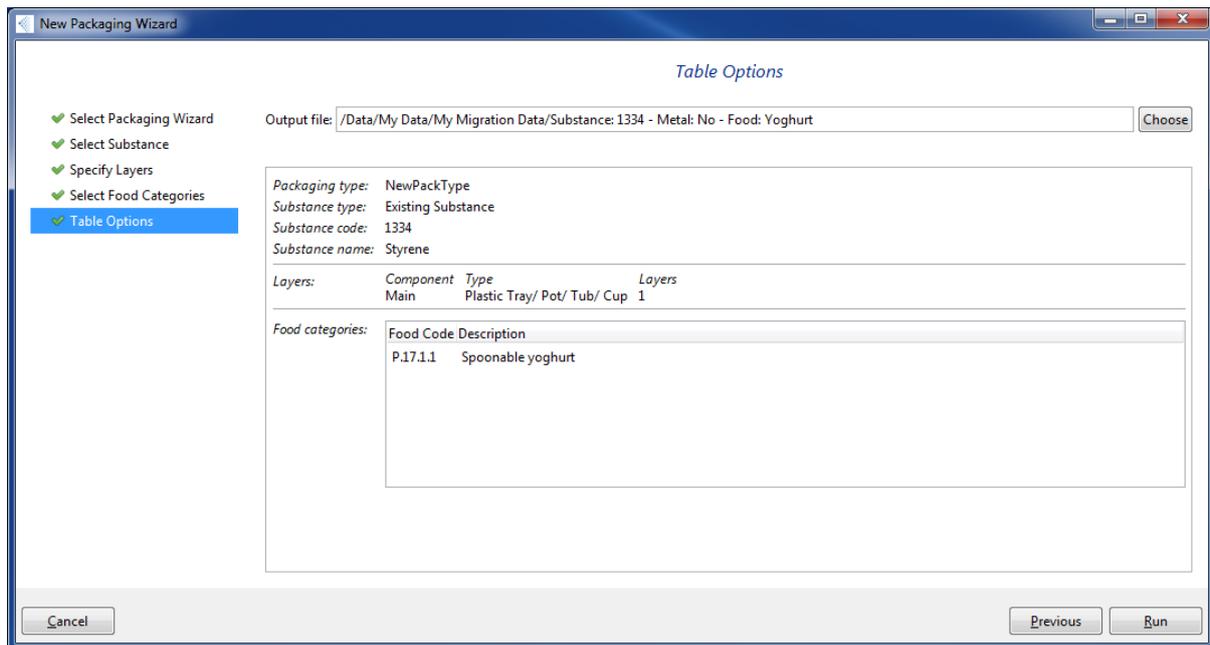


Figure 3-80: Table Options

Upon completion the user is informed that the assessment has come to an end. This is shown in Figure 3-81.

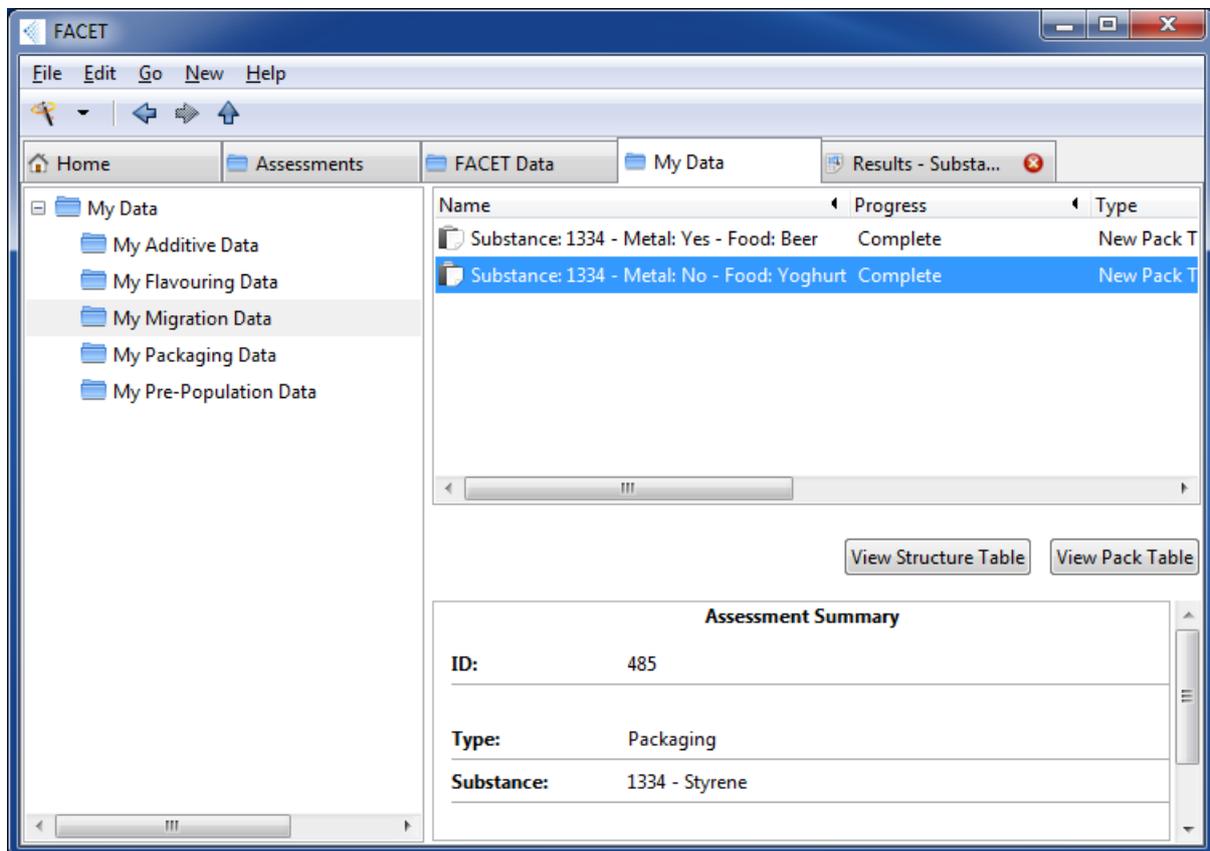


Figure 3-81: Assessment Complete

Now the user can run an assessment on the table created in the previous assessment. This calculation is illustrated in Figure 3-82 to Figure 3-92.

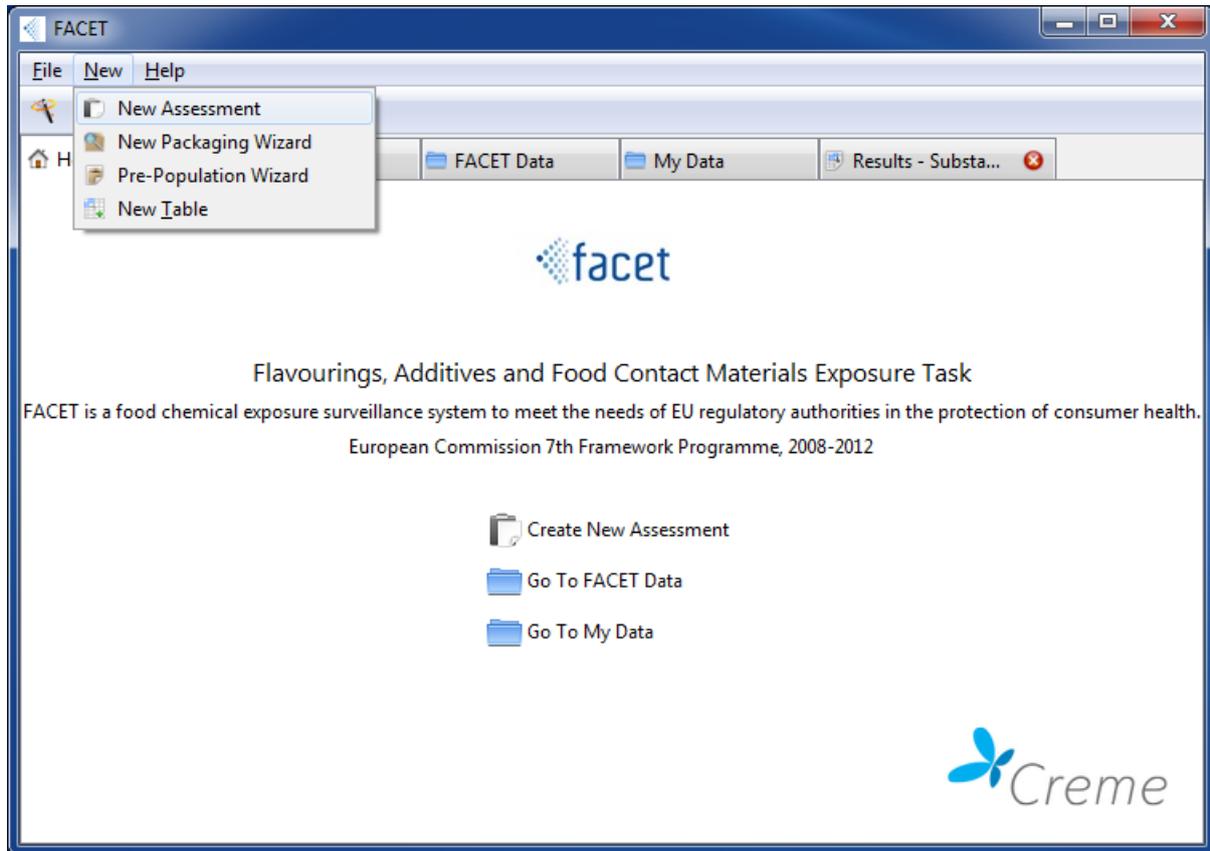


Figure 3-82: Run Assessment

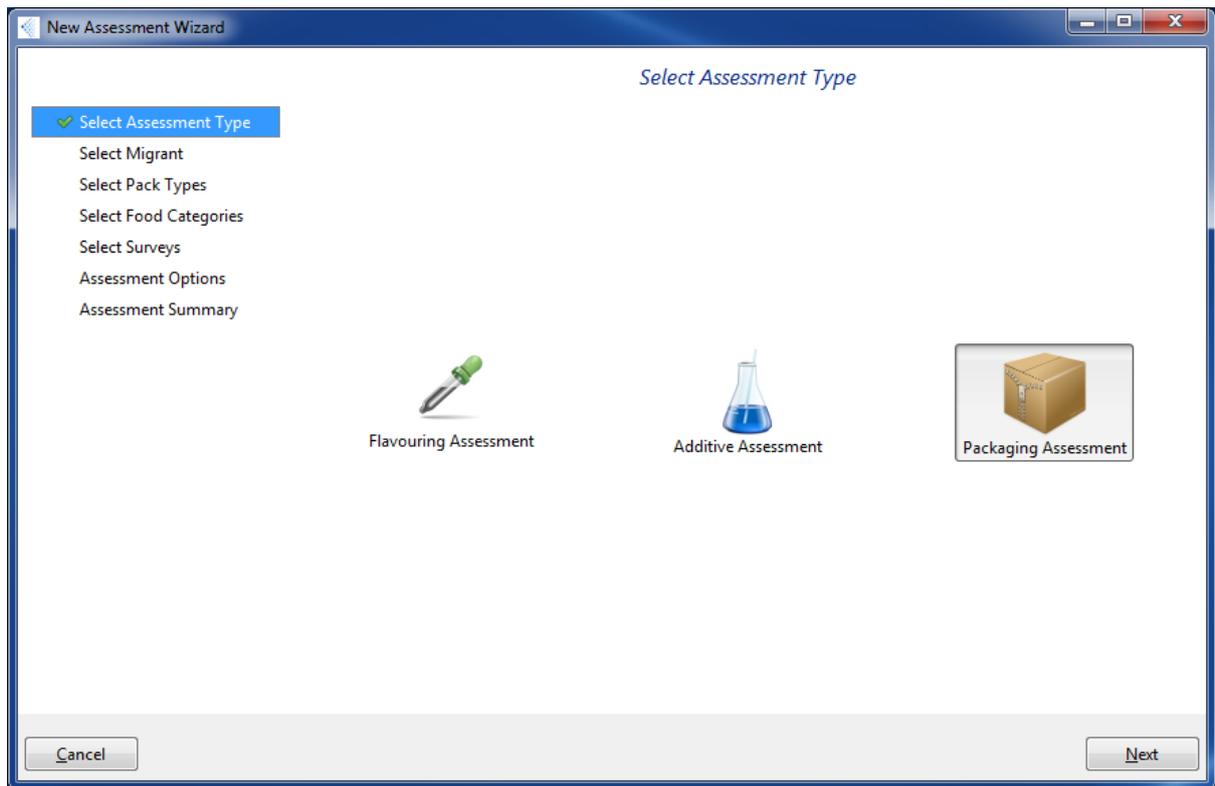


Figure 3-83: Packaging Assessment

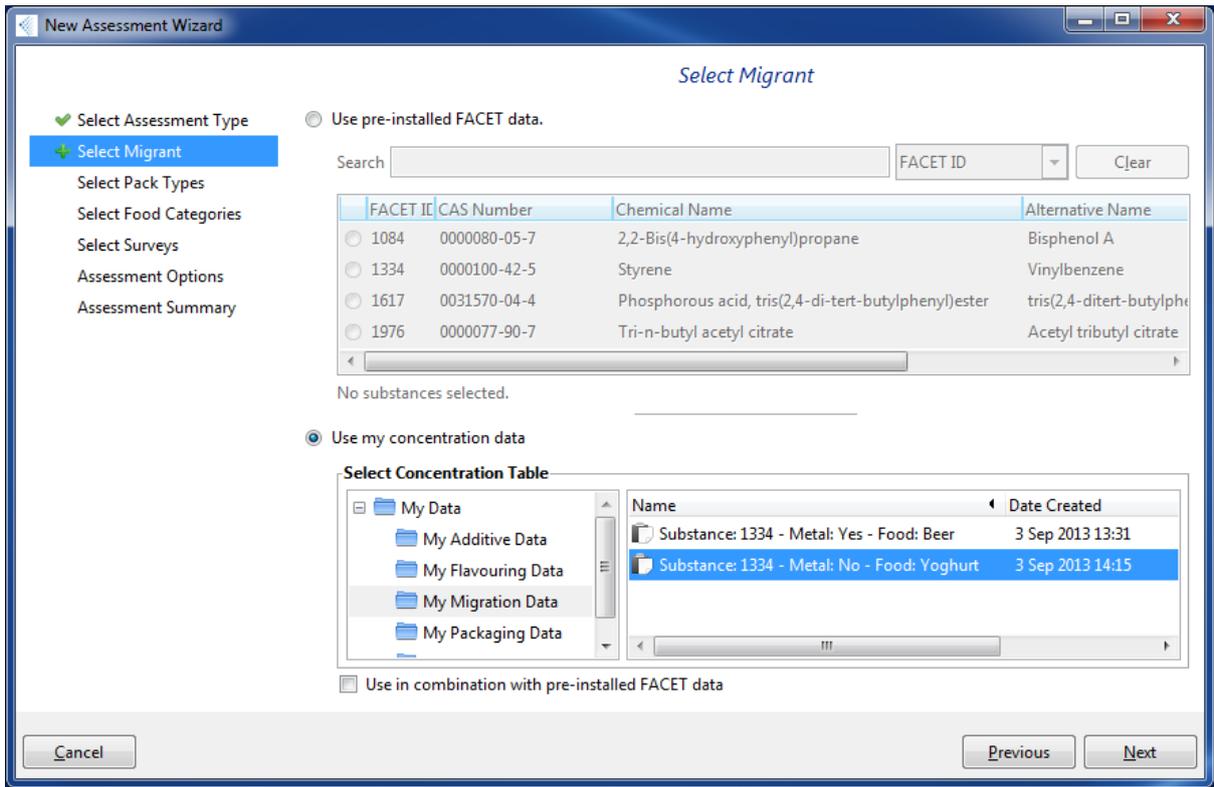


Figure 3-84: Select Table

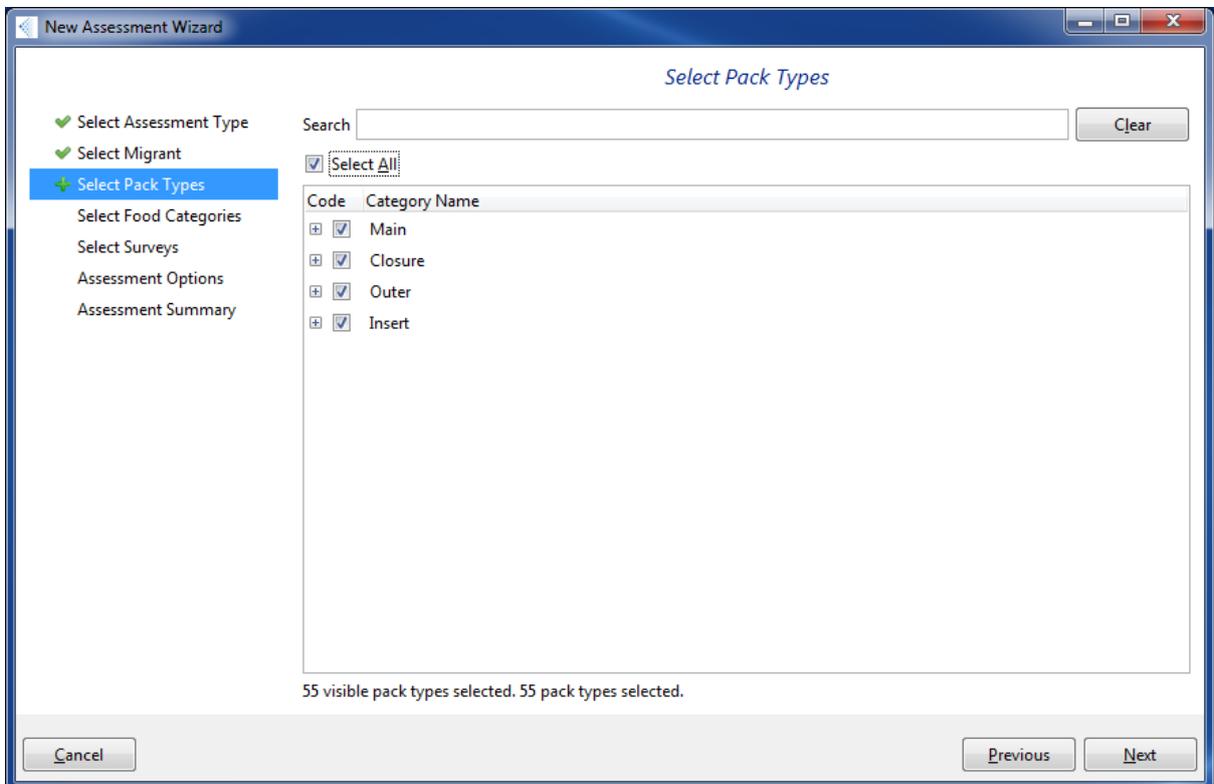


Figure 3-85: Select Pack Types

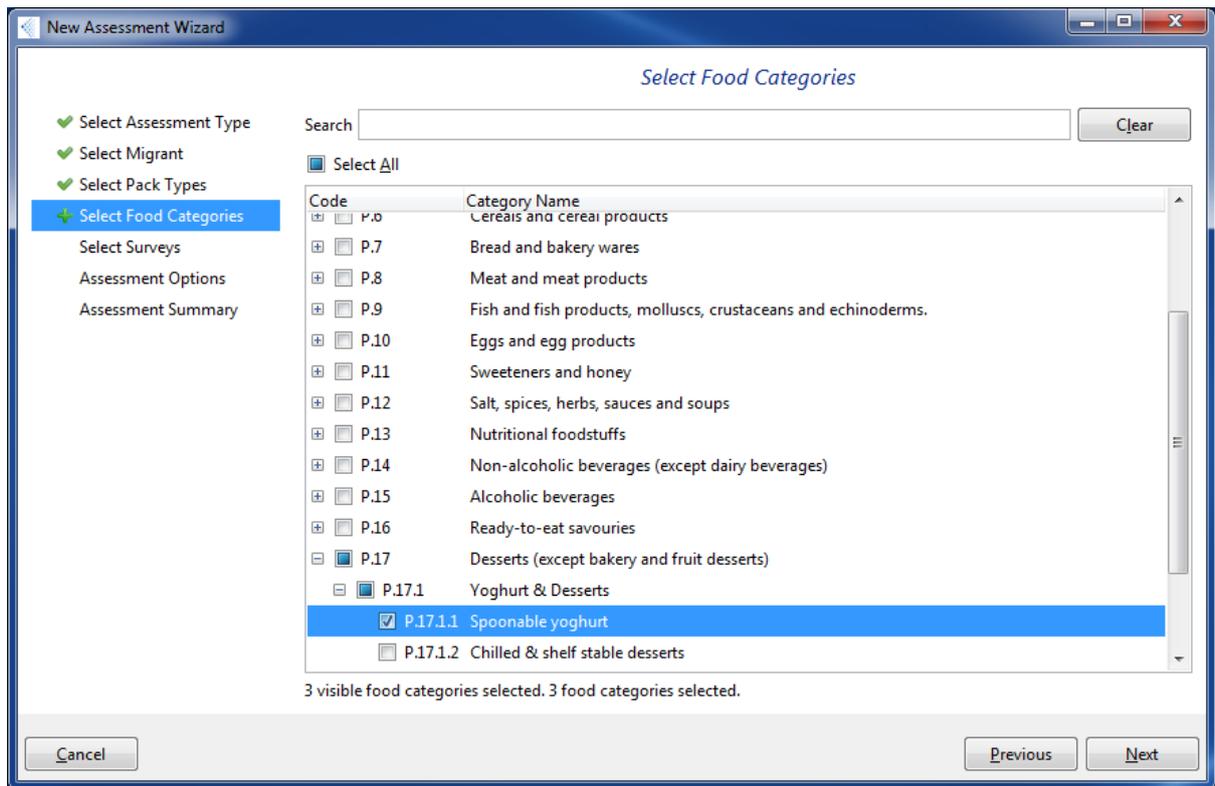


Figure 3-86: Select Food Categories

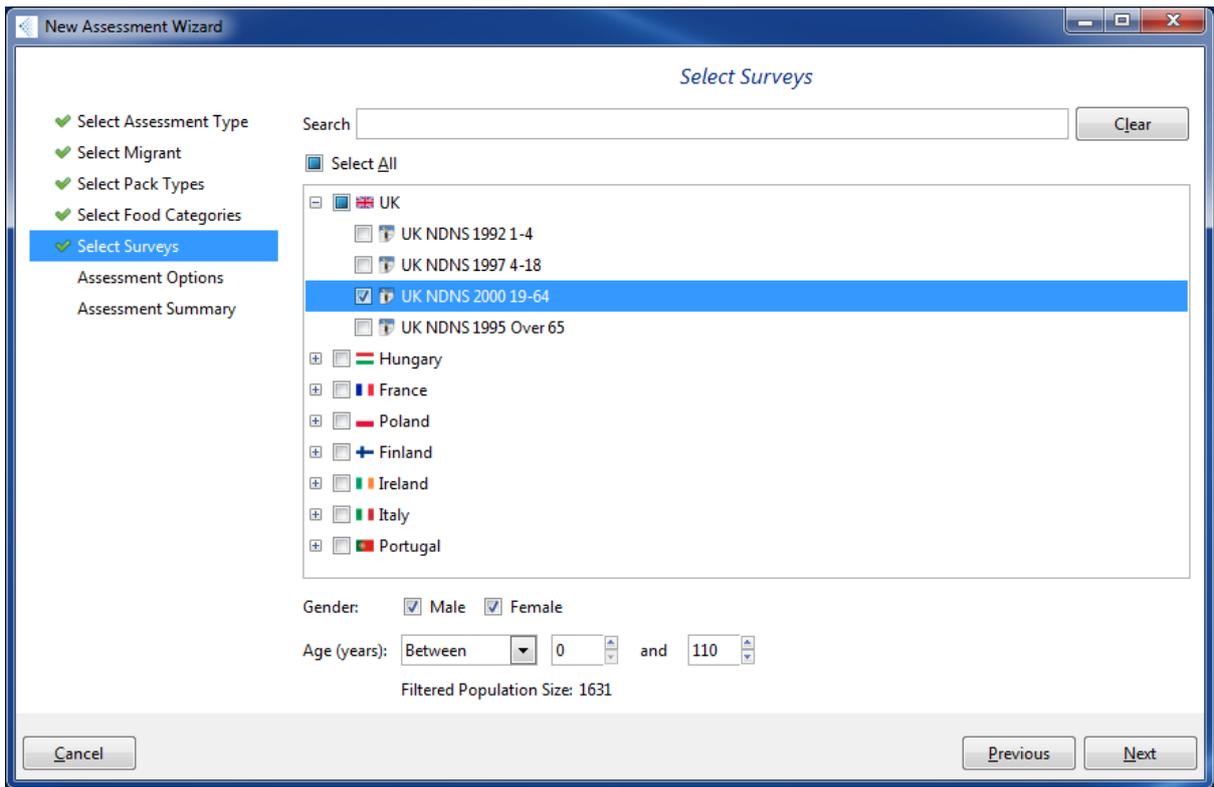


Figure 3-87: Select Survey

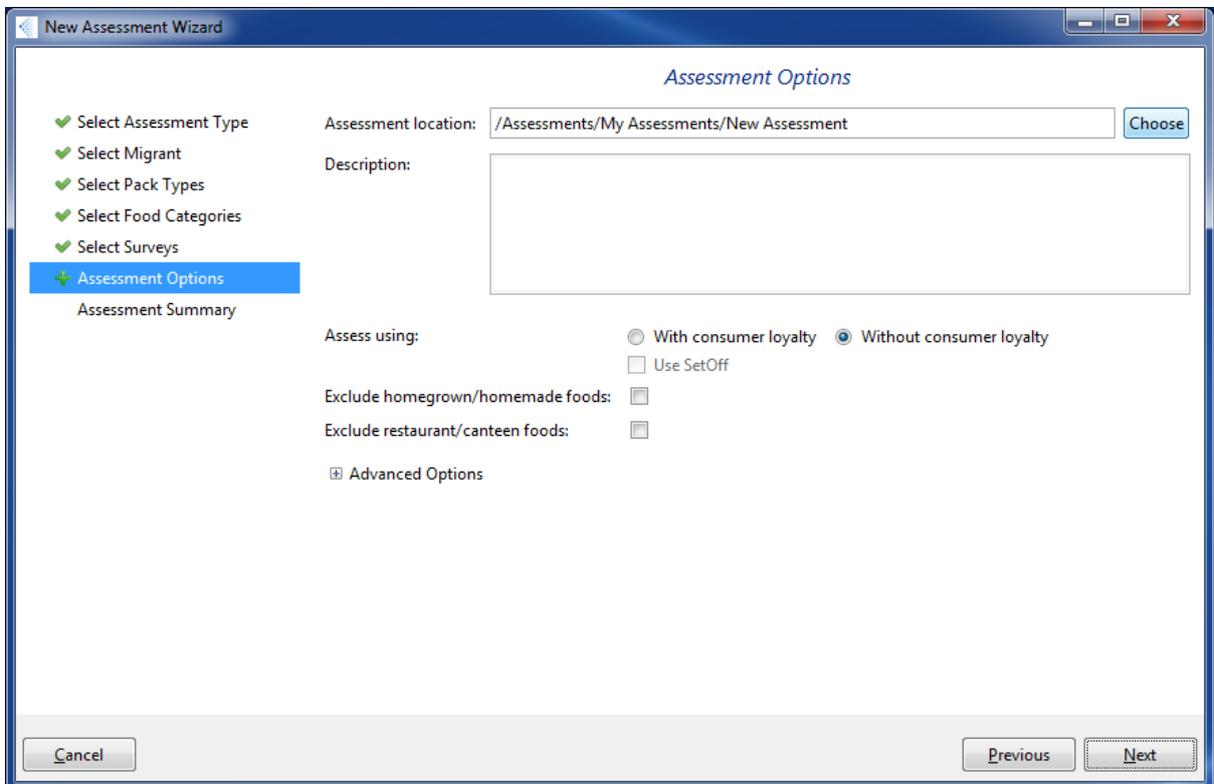


Figure 3-88: Assessment Options

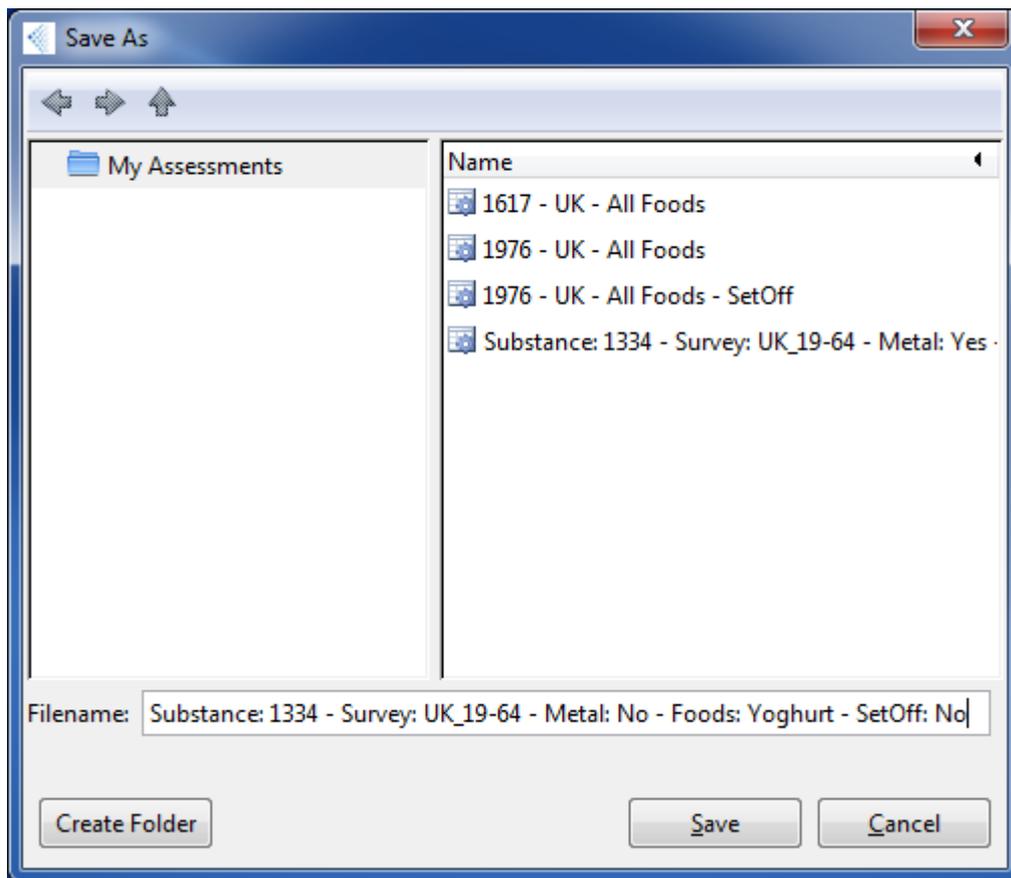


Figure 3-89: Naming Table

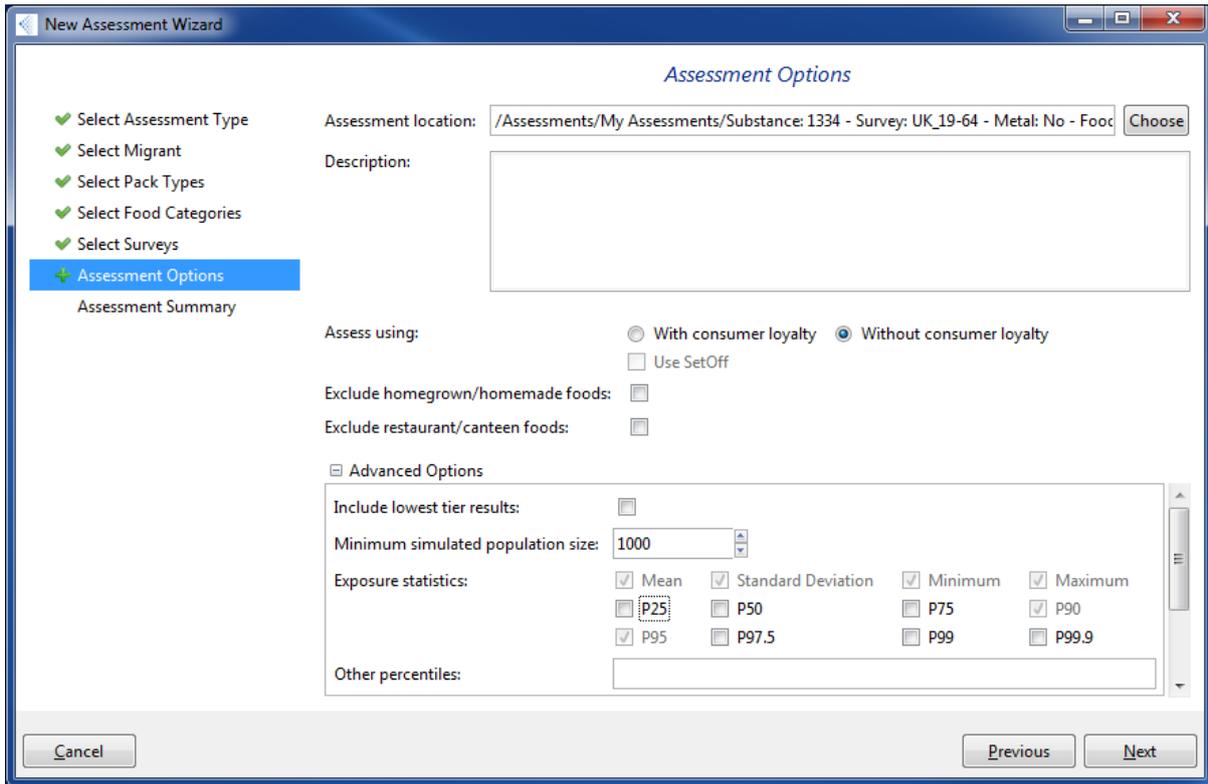


Figure 3-90: Advanced Options

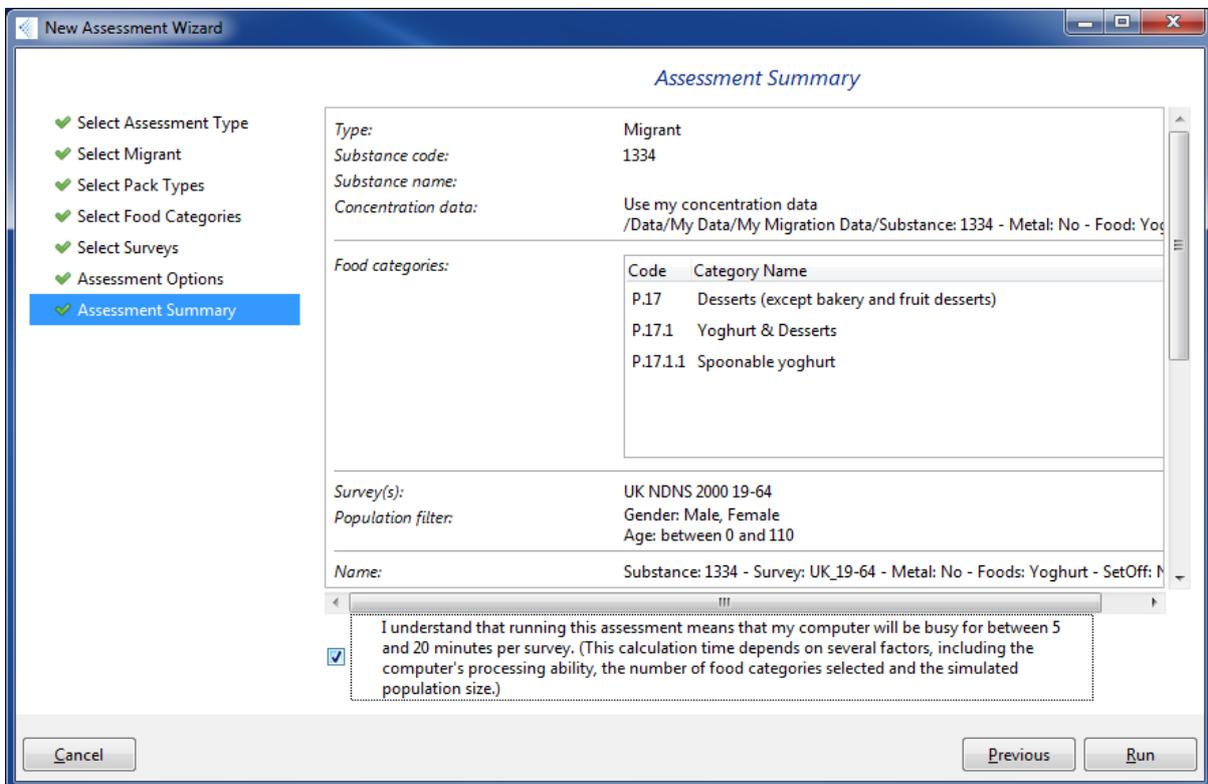


Figure 3-91: Summary of Assessment

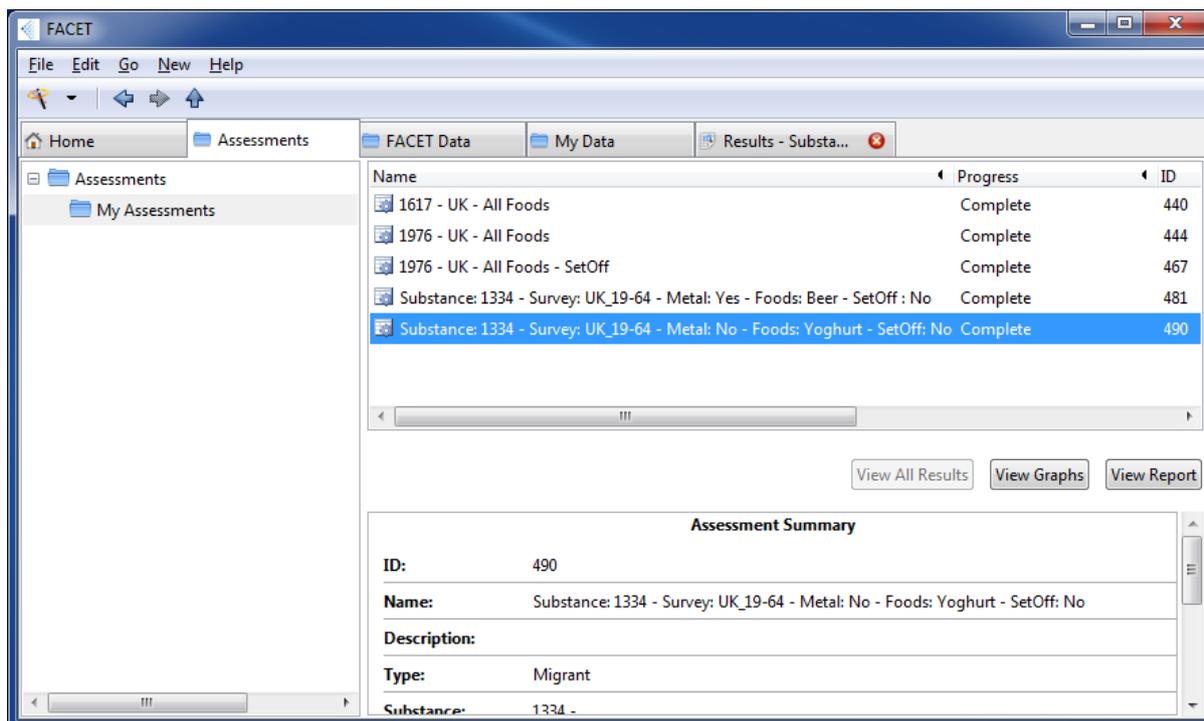


Figure 3-92: Assessment Complete

After completion, the user can now view the data in a report format or else visually using graphs. This is shown in Figure 3-93 to Figure 3-95.

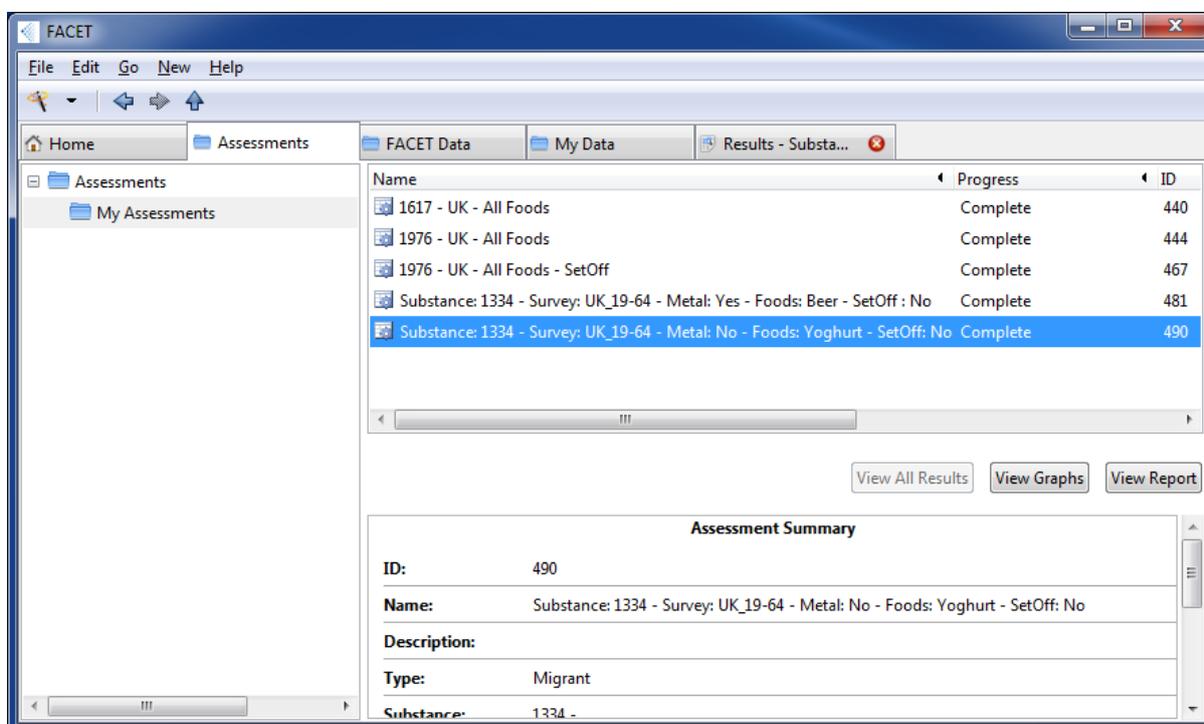


Figure 3-93: Select View Graphs

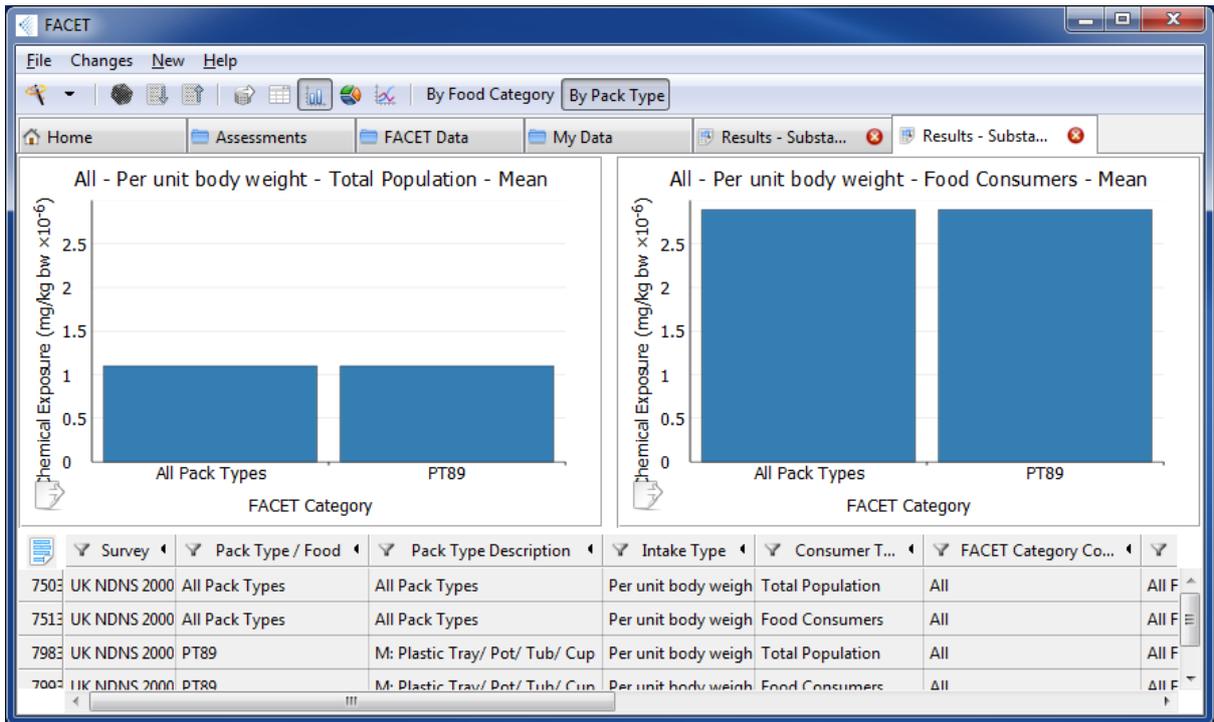


Figure 3-94: Viewing Graphs, by Pack Type

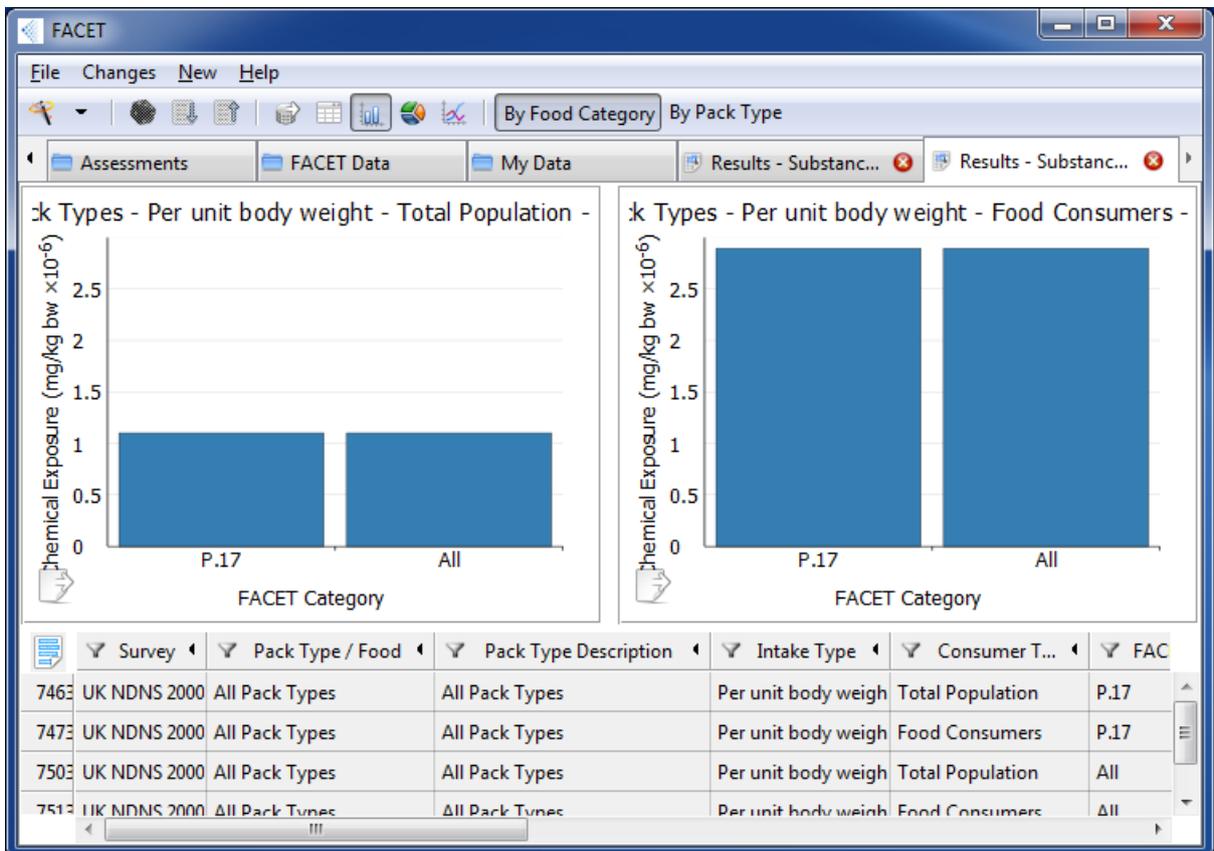


Figure 3-95: Viewing Graphs, by Food Category

### 3.3.3 Using the New Packaging Wizard for a New Substance

Another option in the software is for the user to enter a new substance and then run a packaging assessment for the substance. To enter a new substance, the user initially selects the “New Packaging Wizard” as shown in Figure 3-96.

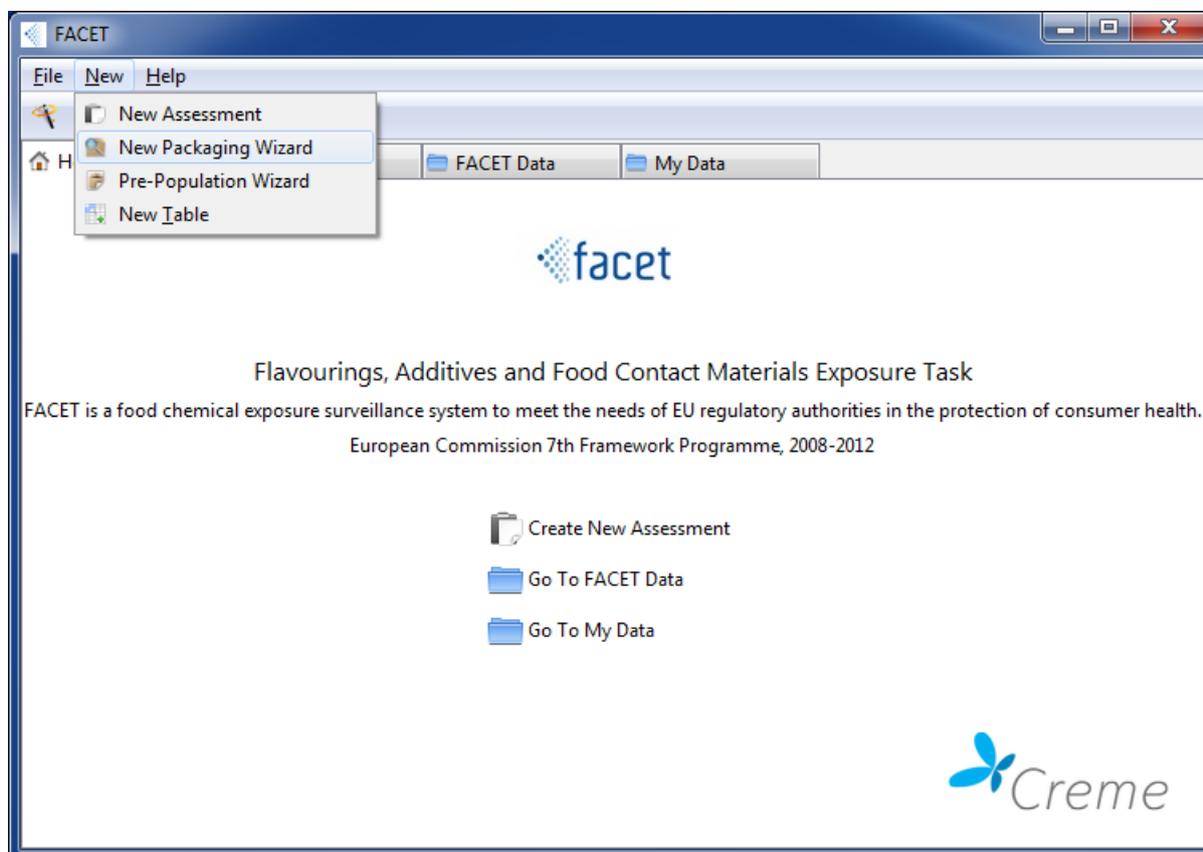


Figure 3-96: New Packaging Wizard

The user has the option of selecting a Non-Metal or Metal pack type. In this example, we select a “New Metal Pack Type”.

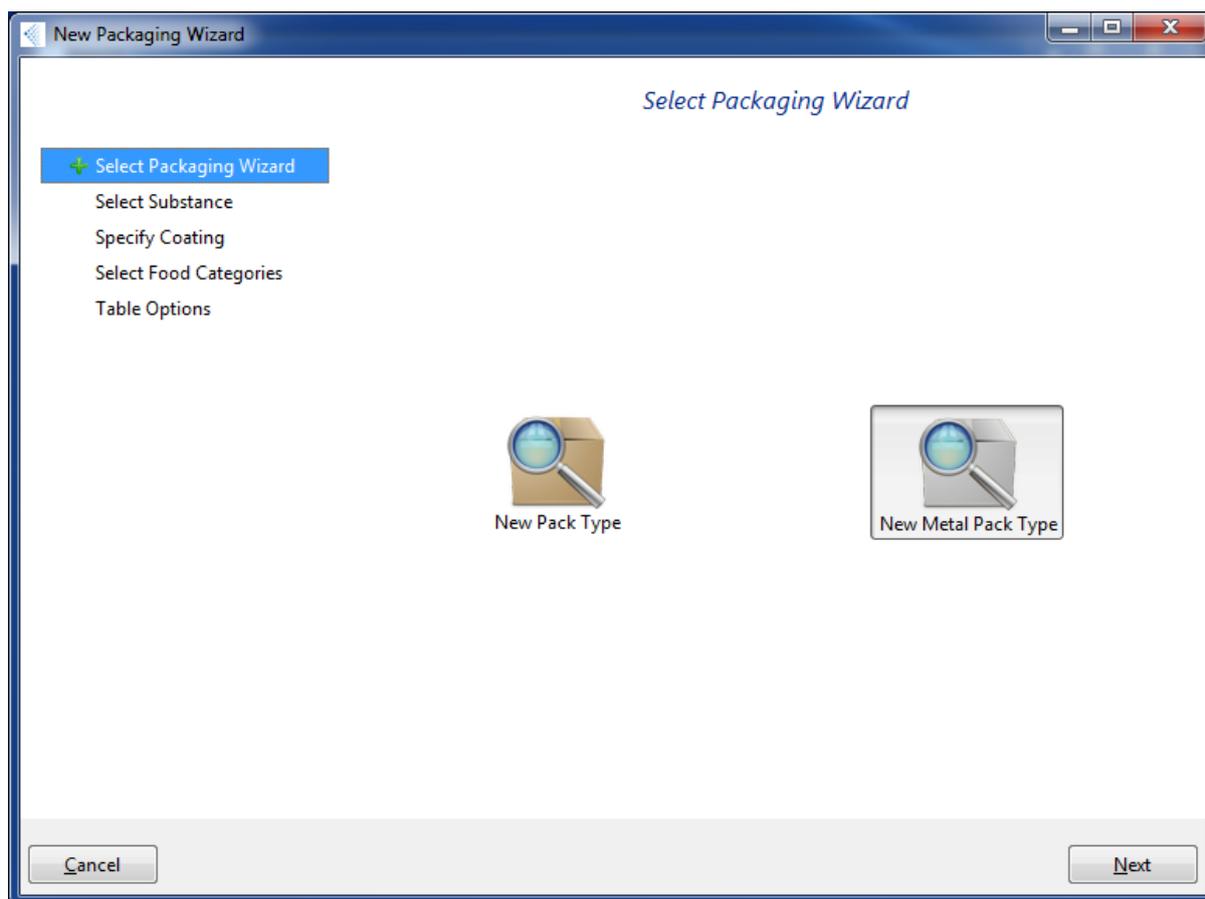


Figure 3-97: New Metal

At this stage, a new substance can be used by entering the appropriate information as is done in Figure 3-98. A suitable “Substance Name” is required as well as “Log(P)” and “Molecular Weight” details for the substance.

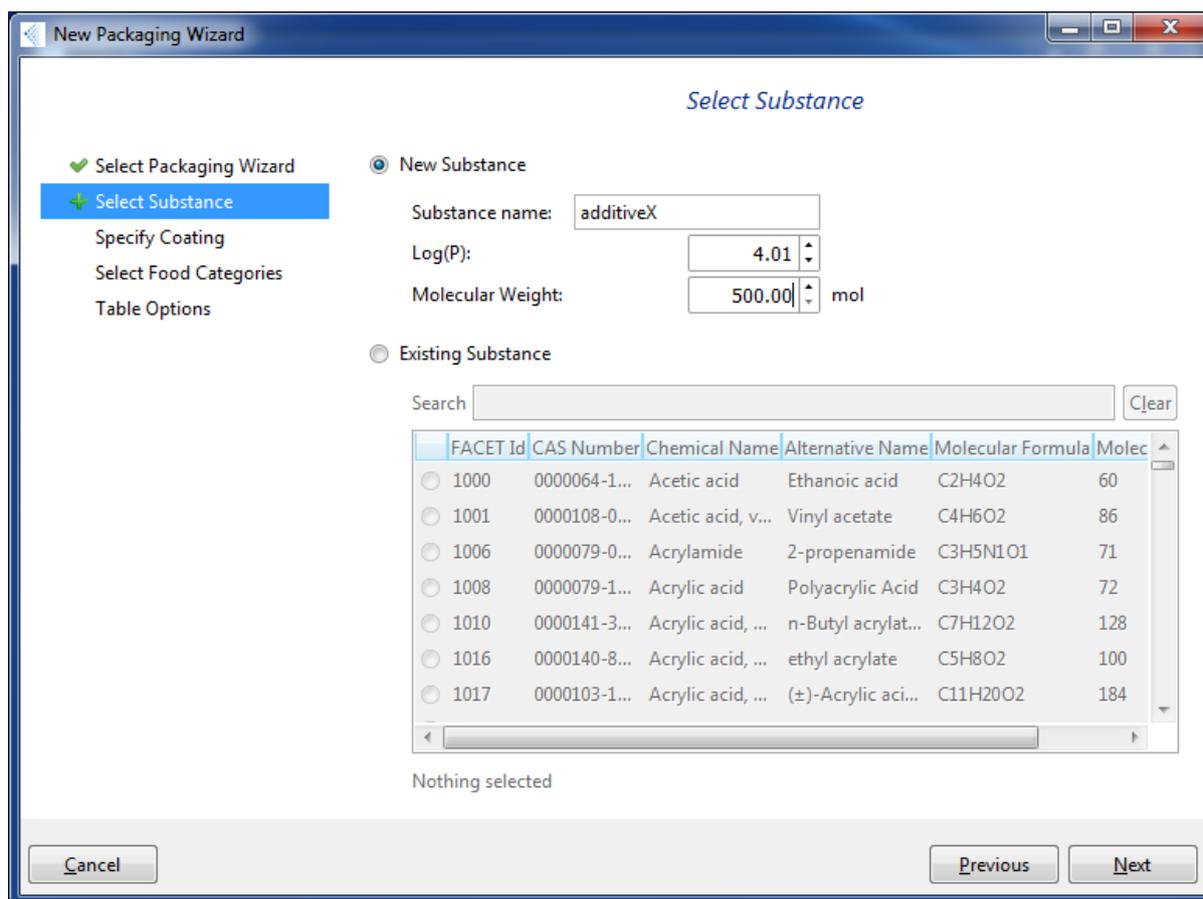


Figure 3-98: New Substance

Once the information for the new substance has been entered, the user can follow a similar approach to that taken in Section 3.3.1 where the concentration of the substance in a specified pack type in a particular food is determined. These steps are illustrated in Figure 3-99 to Figure 3-105.

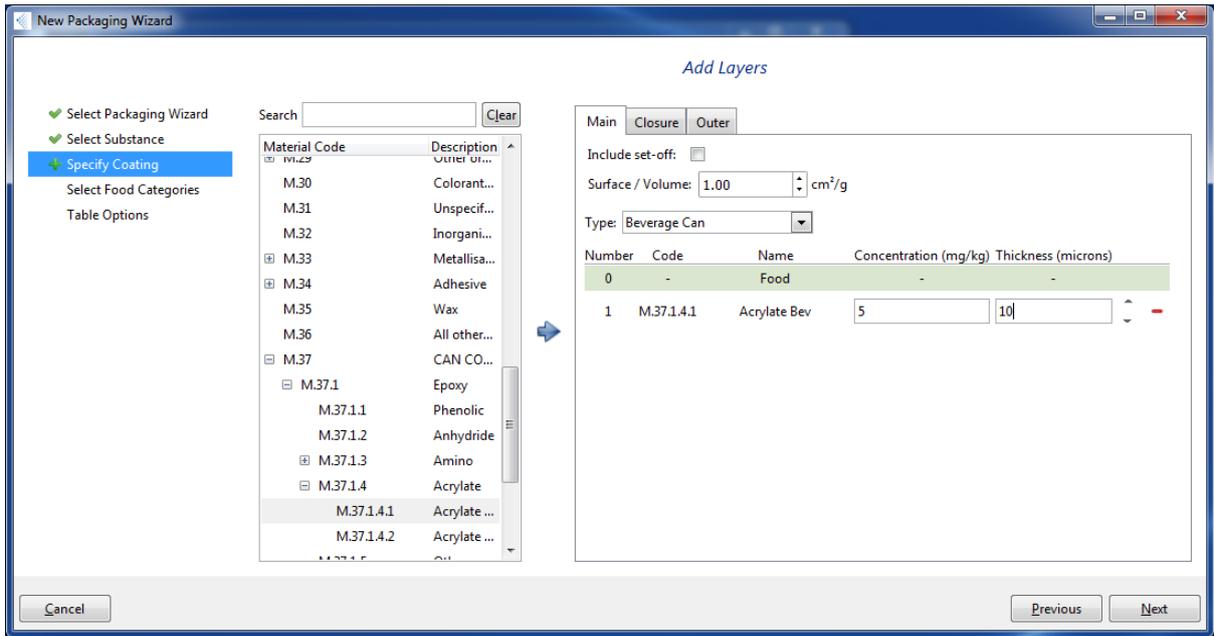


Figure 3-99: Add Layers

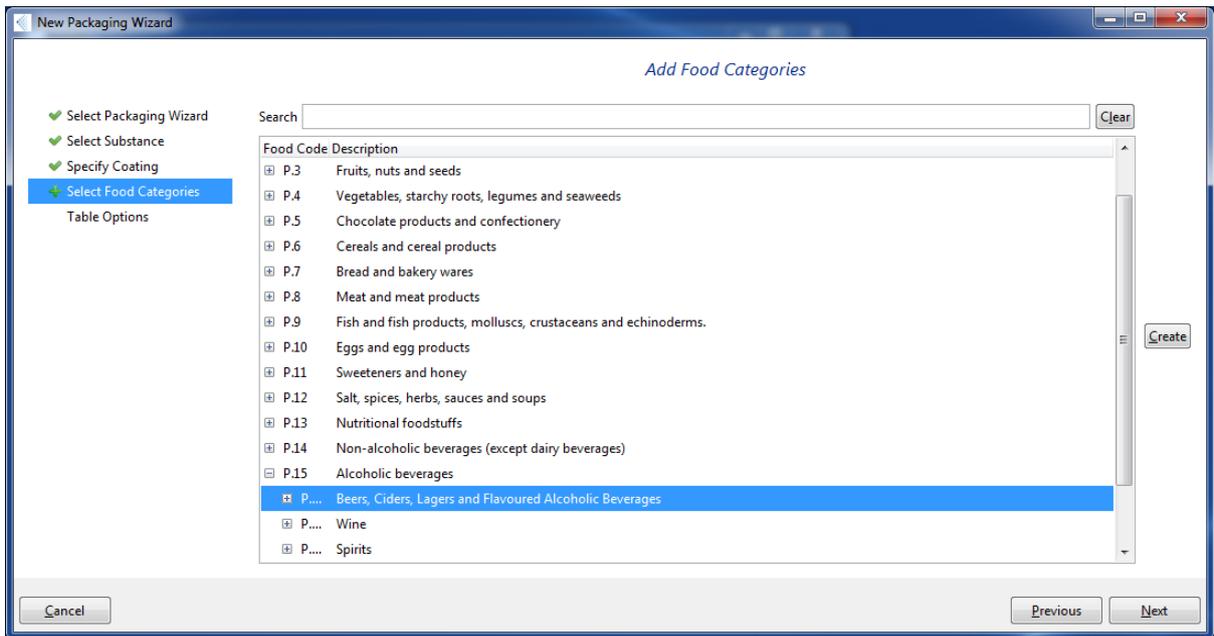


Figure 3-100: Add Food Categories

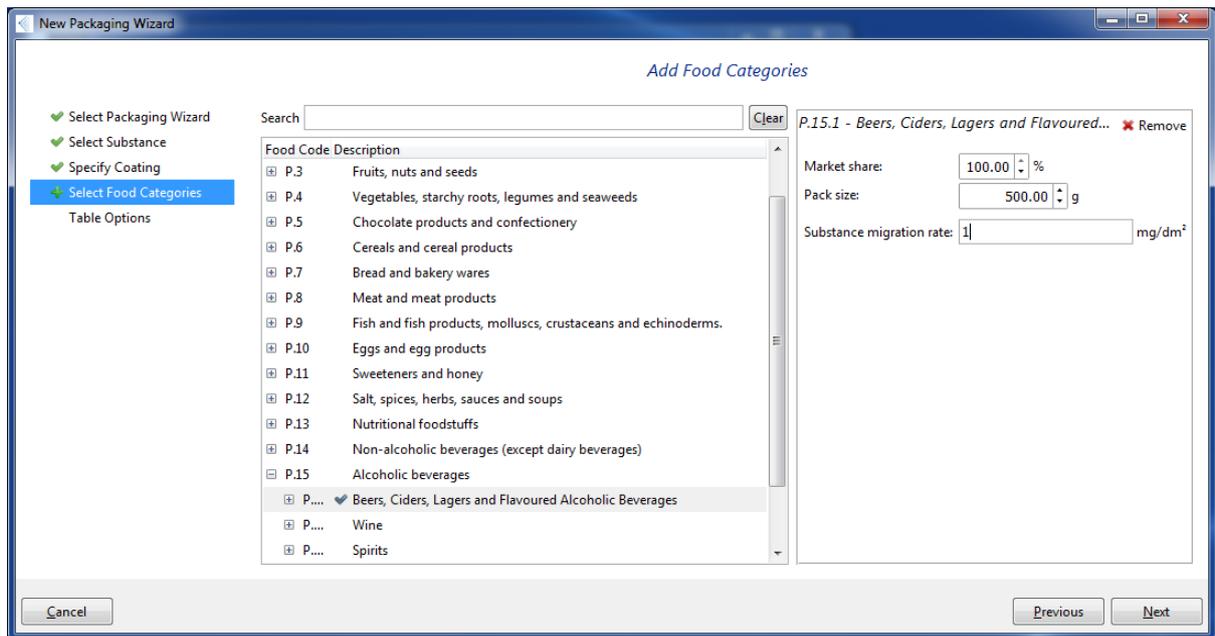


Figure 3-101: Pack Size and Substance Migration Rate

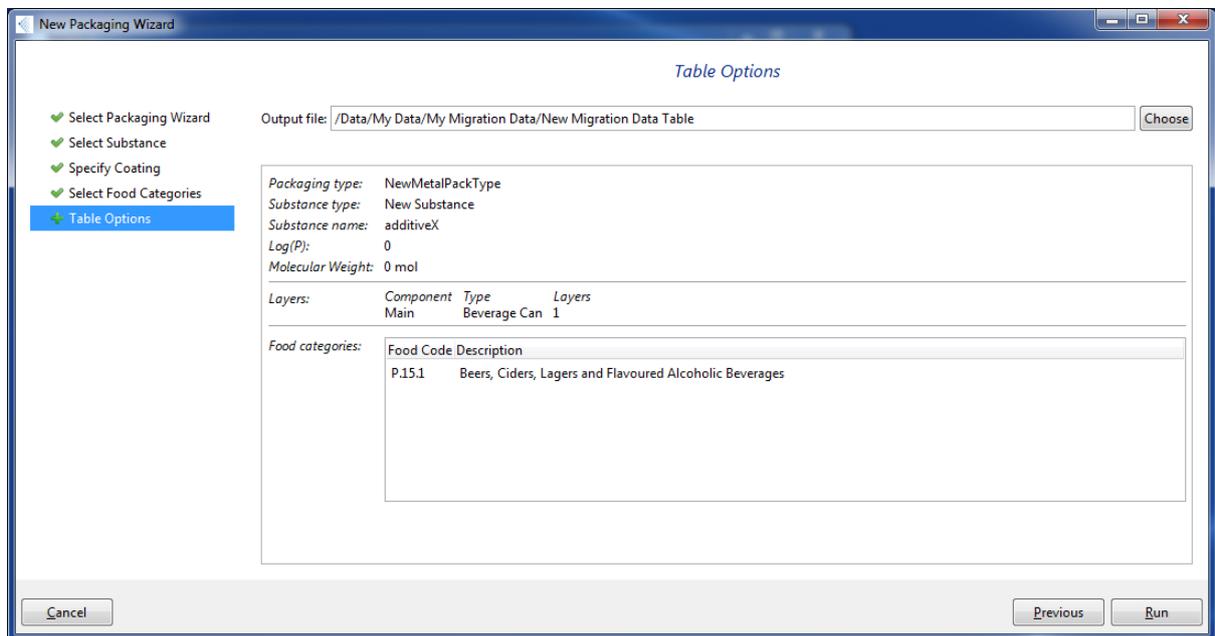


Figure 3-102: Table Options

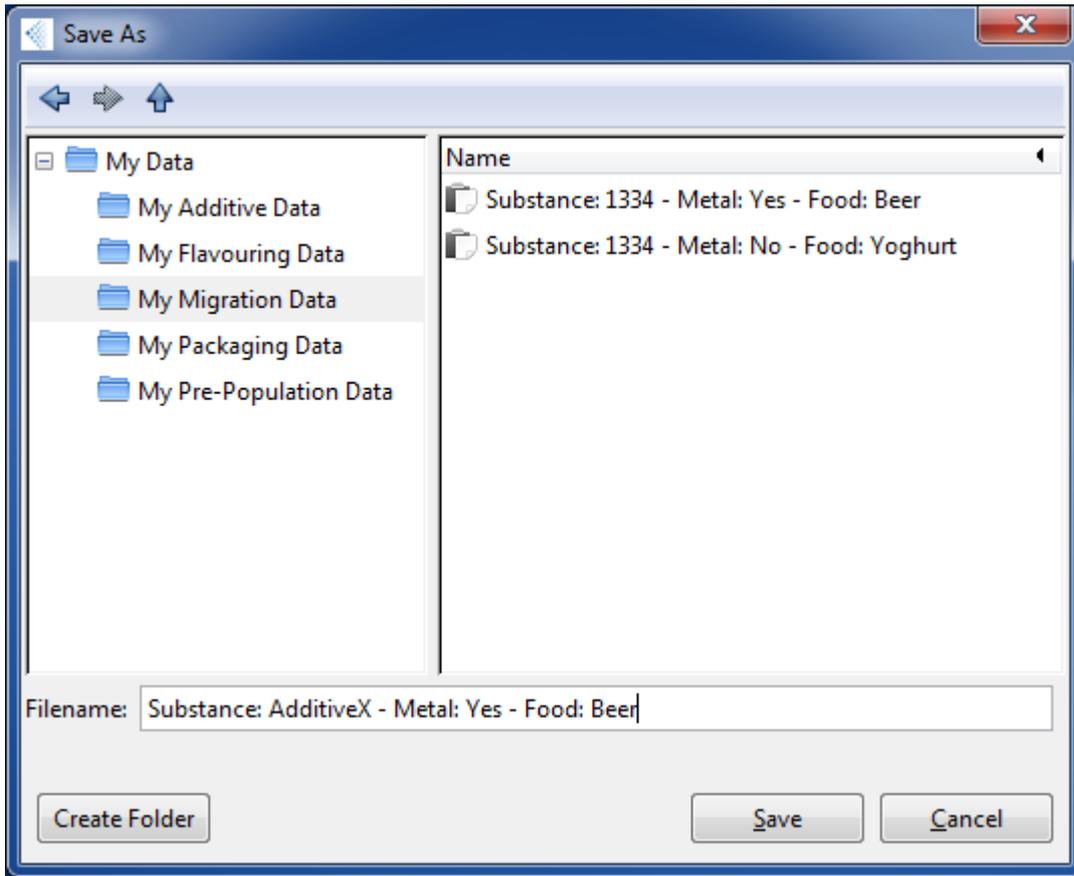


Figure 3-103: Naming Table

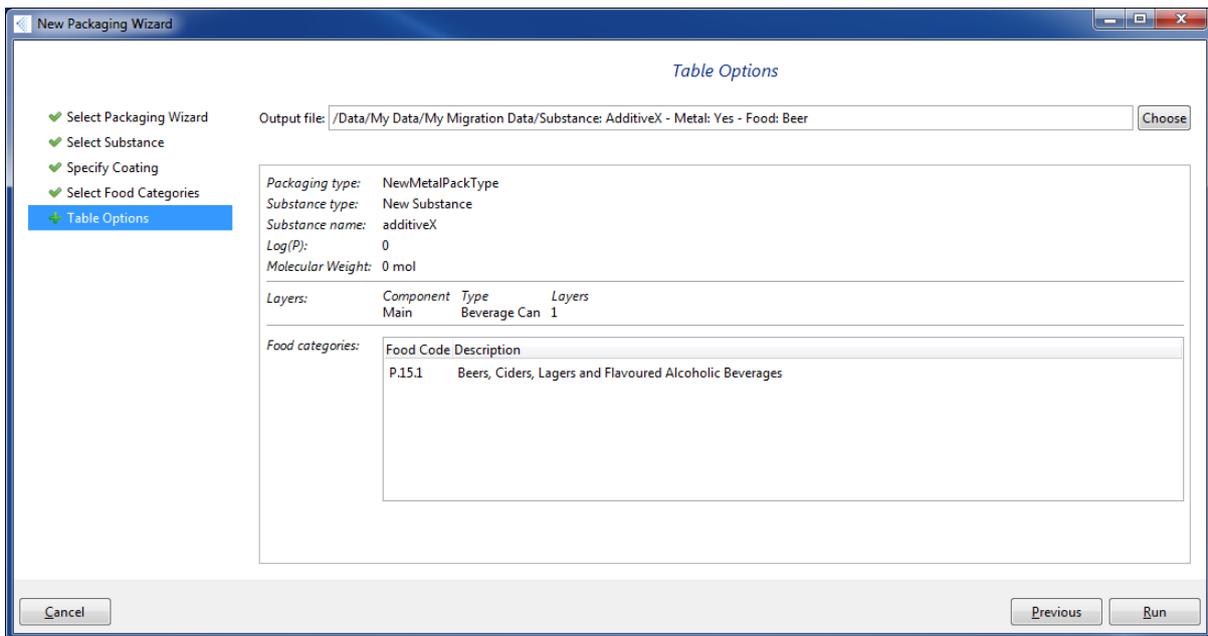


Figure 3-104: Ready to Run

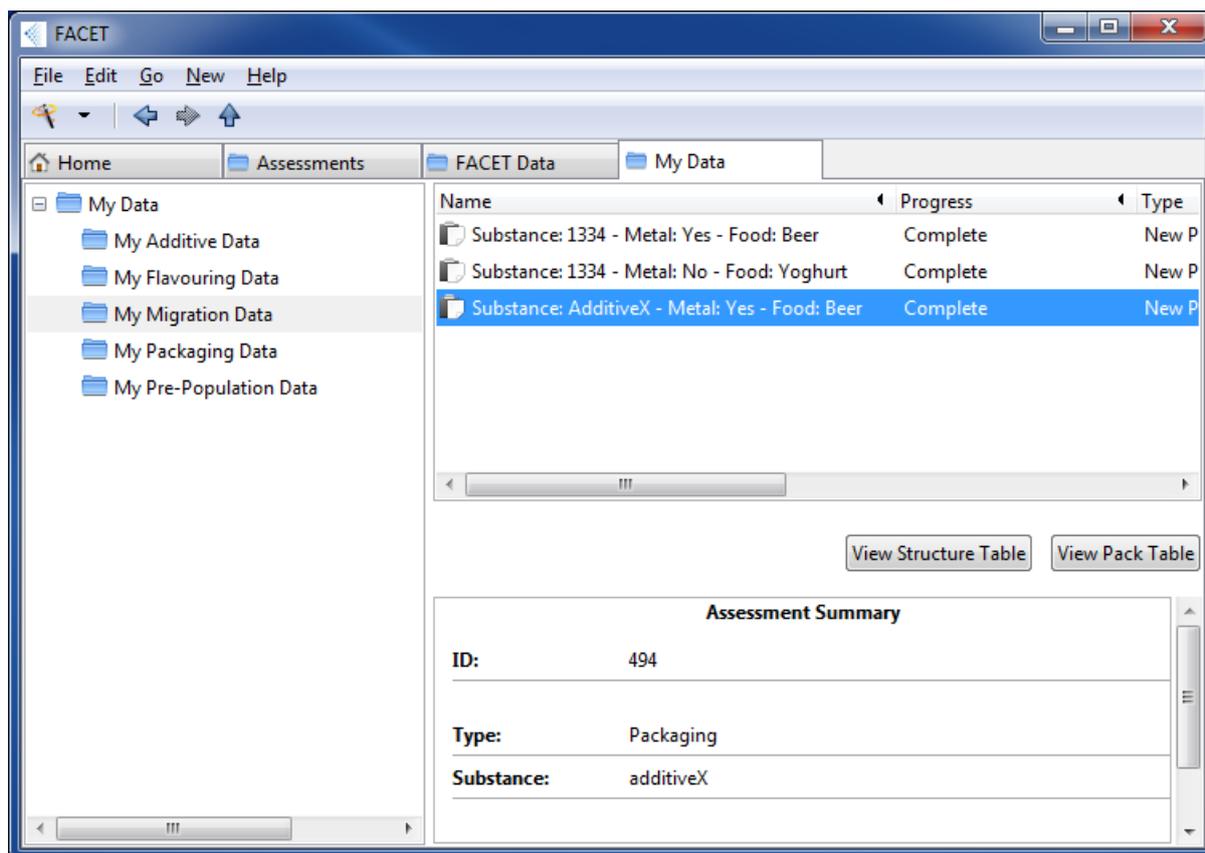


Figure 3-105: Complete

Once the concentration levels are calculated and stored in a table, a packaging assessment can be carried out on the results. This is illustrated in Figure 3-106 to Figure 3-114.

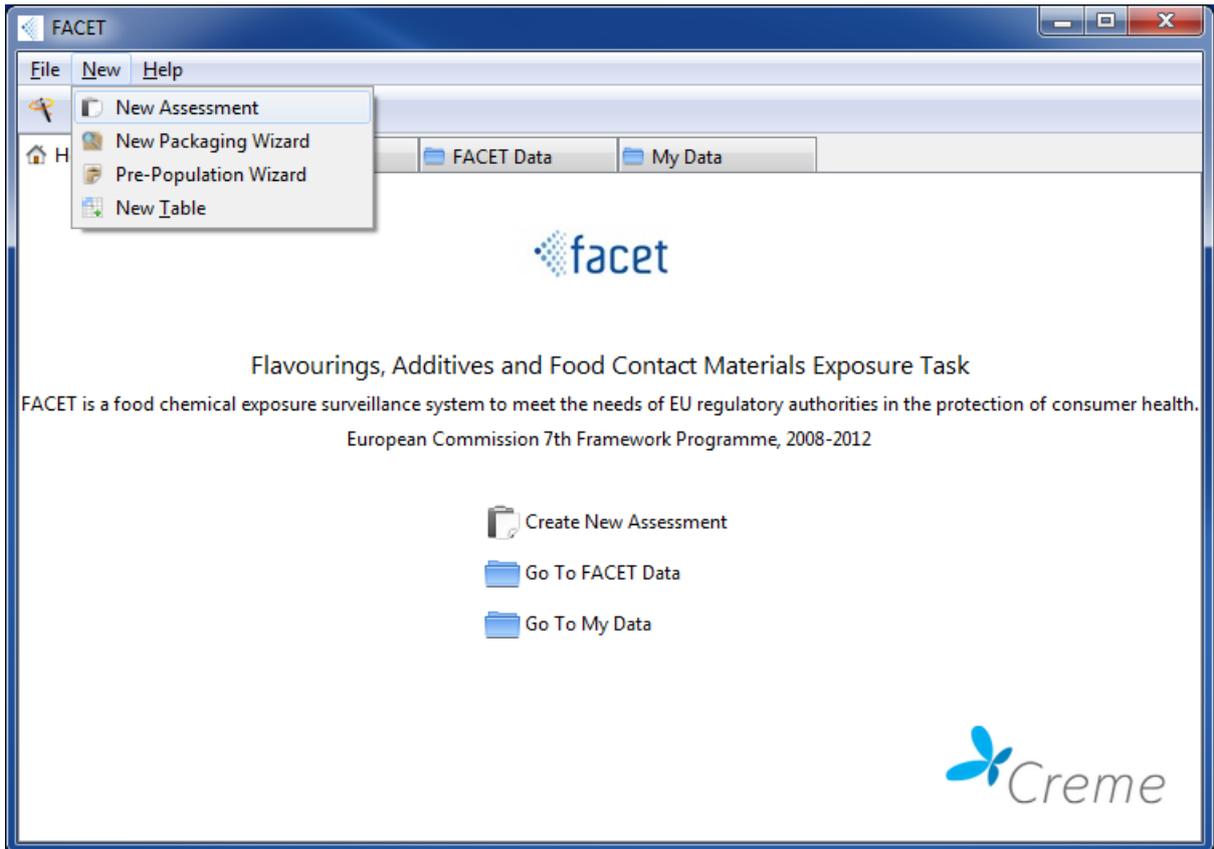


Figure 3-106: New Assessment

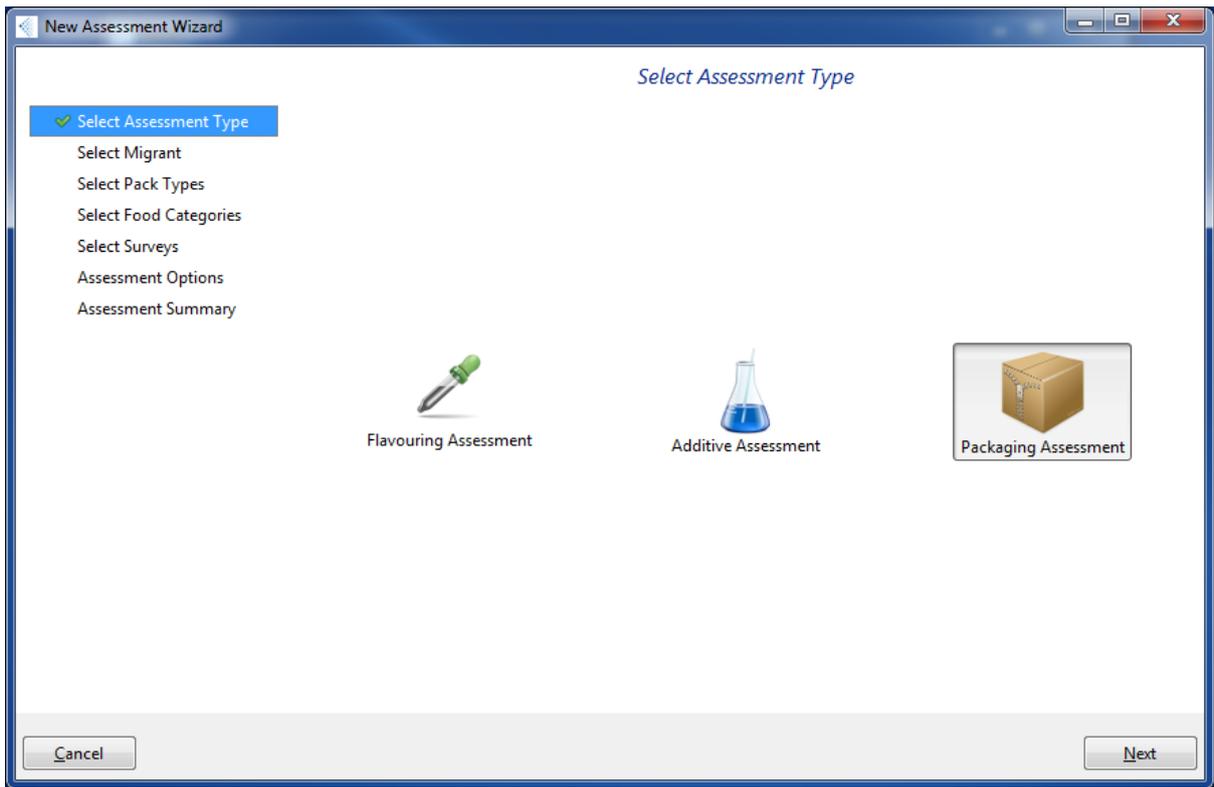


Figure 3-107: Packaging Assessment

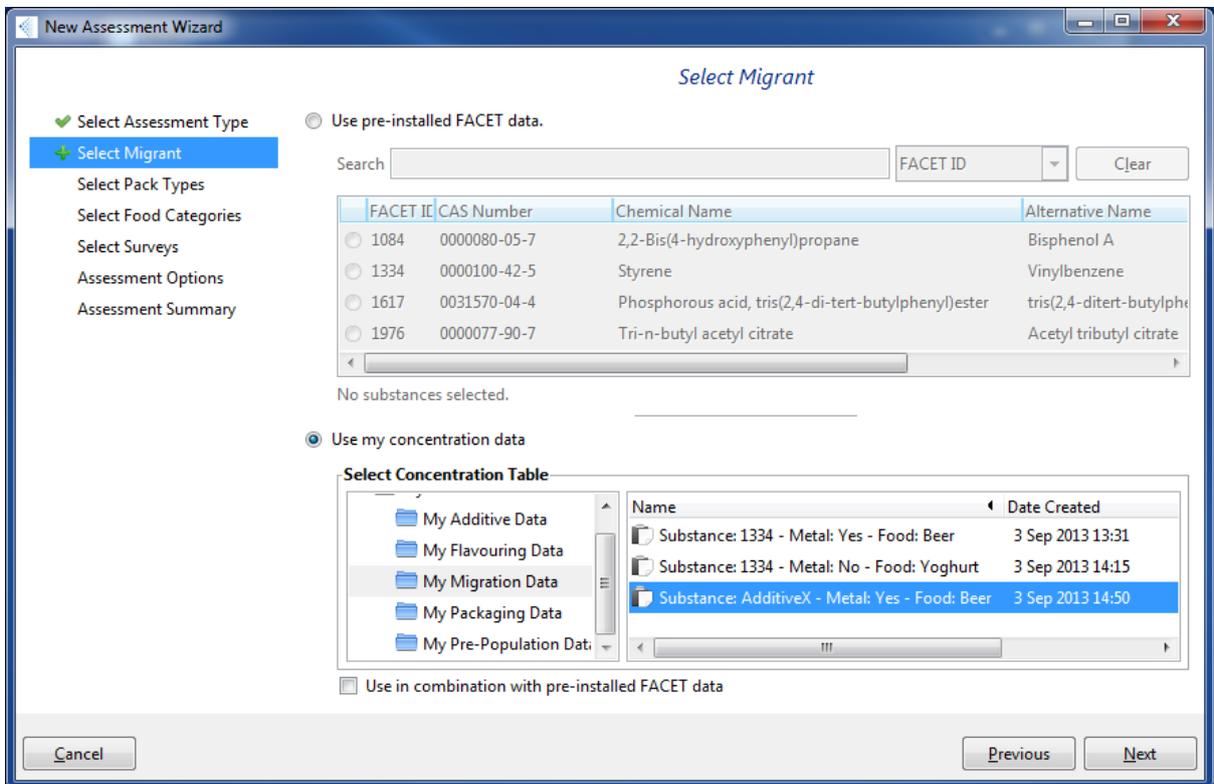


Figure 3-108: Select Table

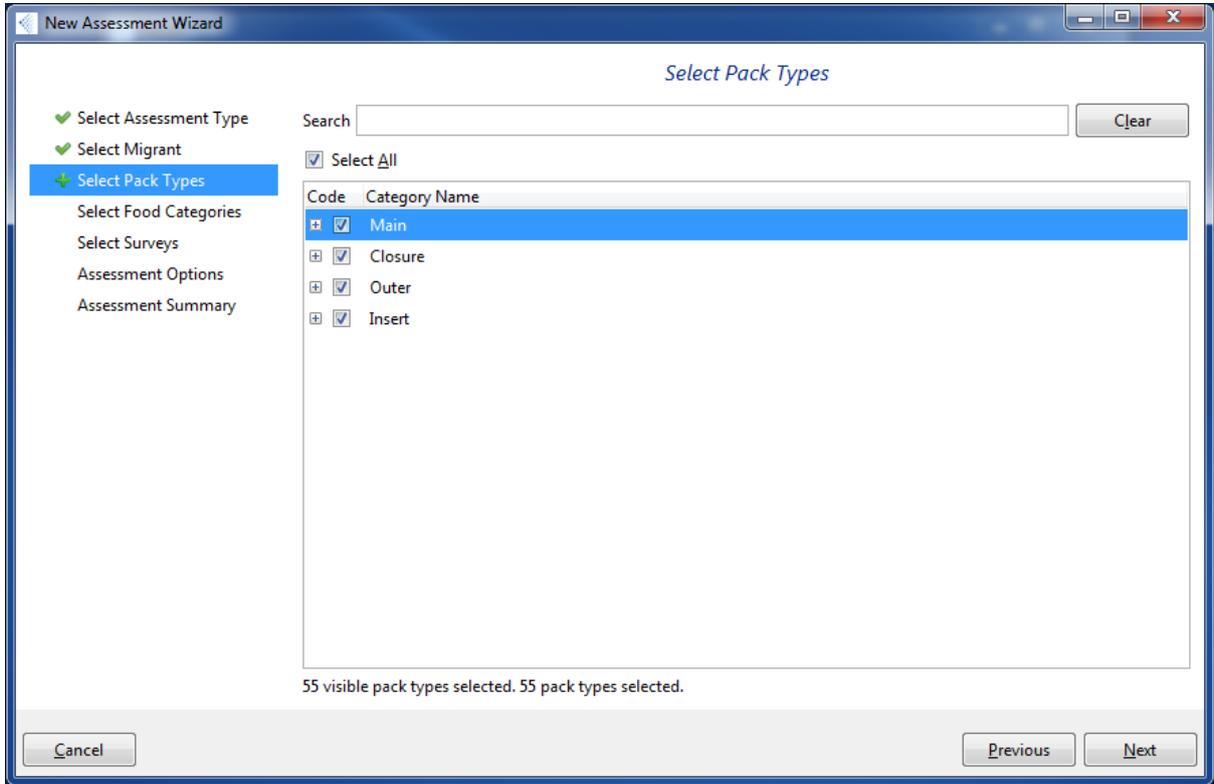


Figure 3-109: Select Pack Types

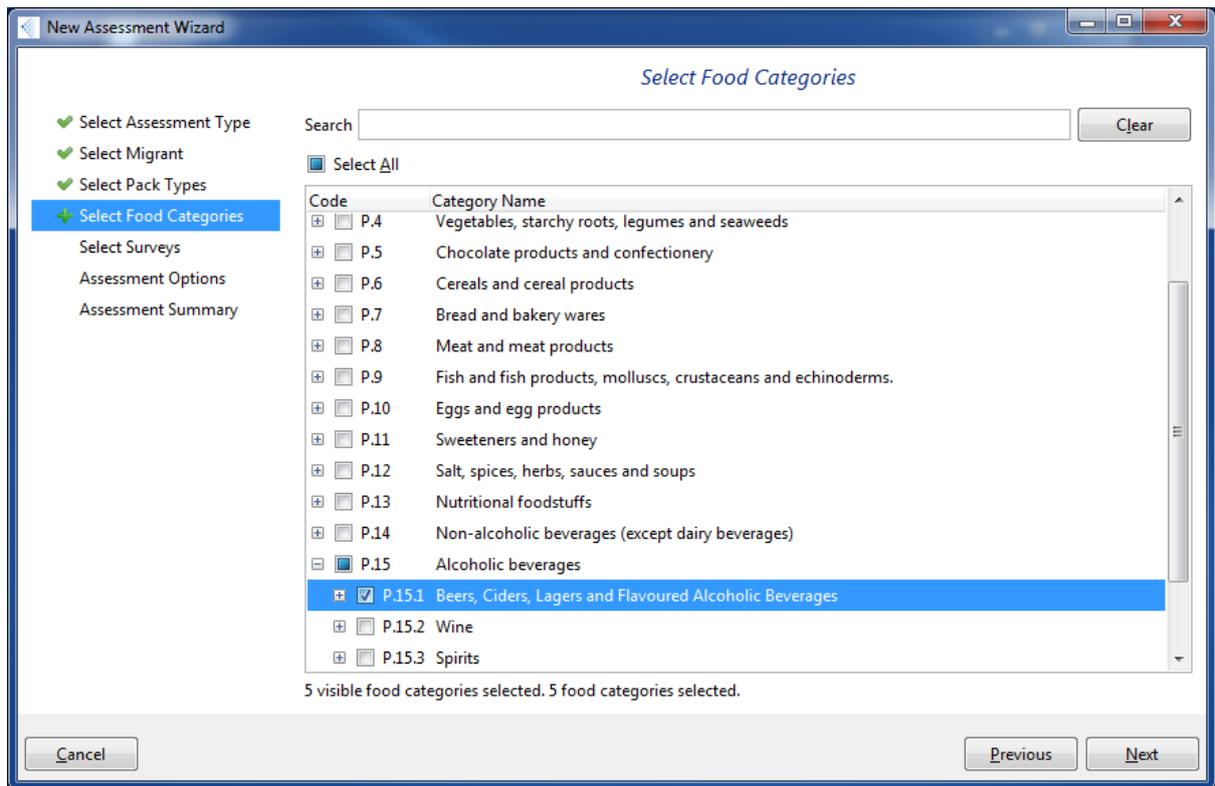


Figure 3-110: Select Food Categories

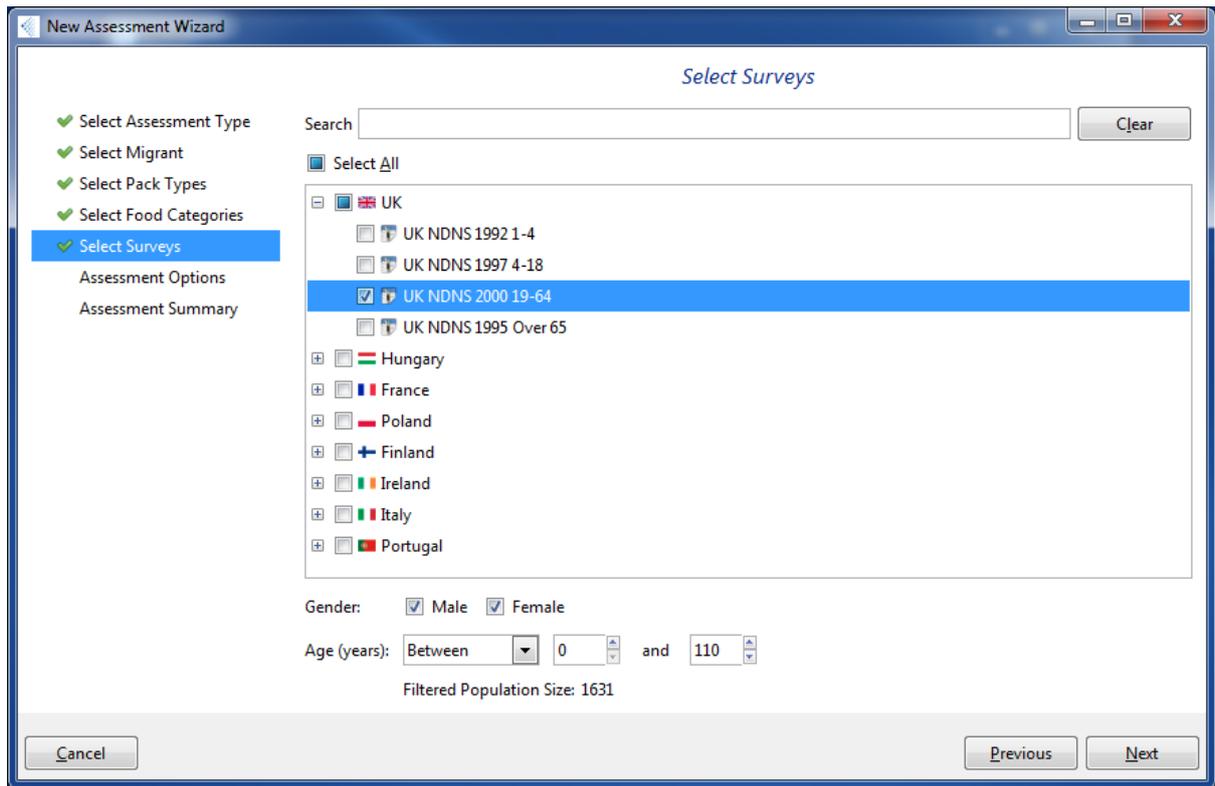


Figure 3-111: Select Survey

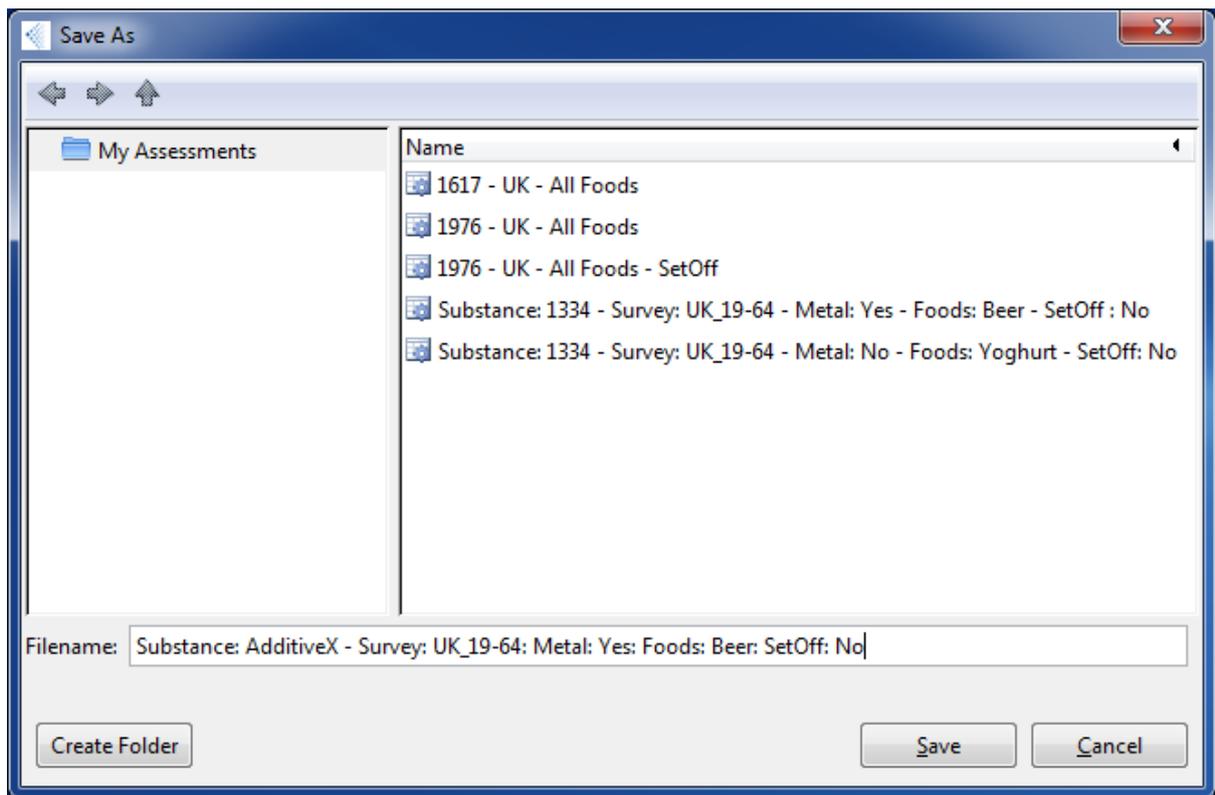


Figure 3-112: Naming Table

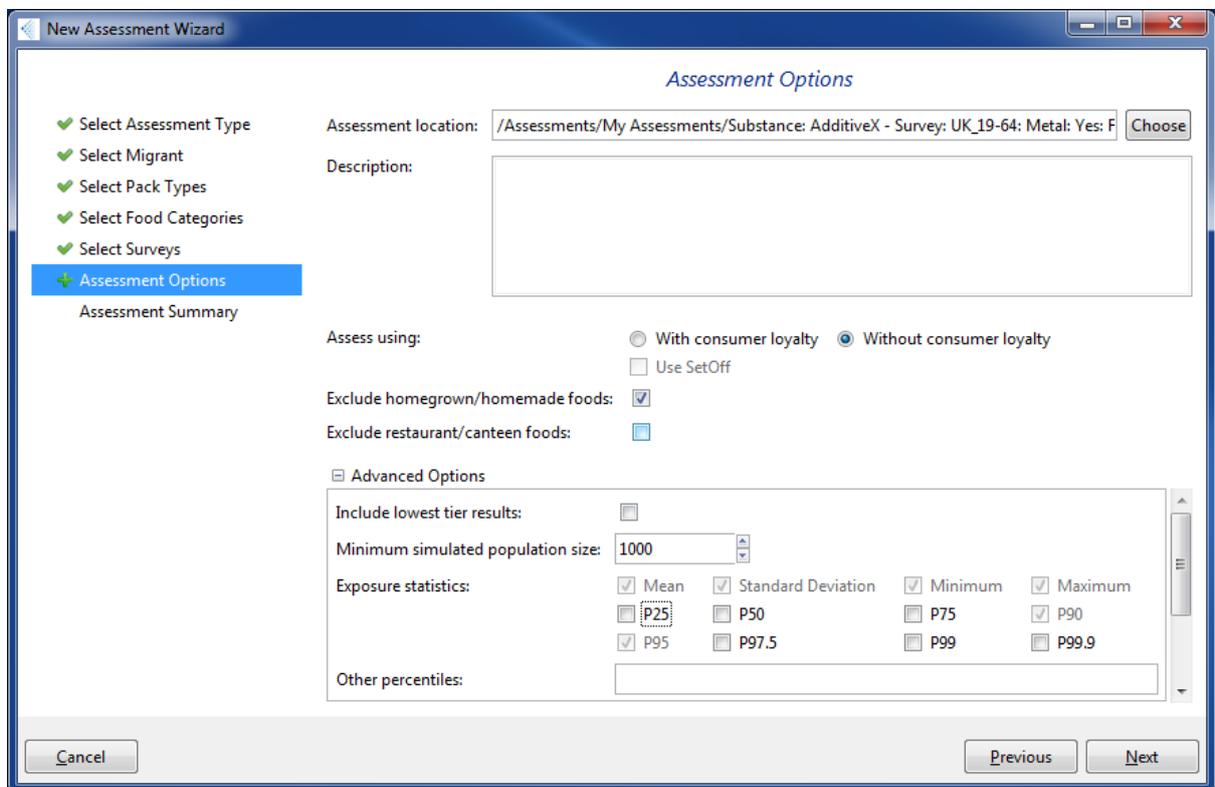


Figure 3-113: Assessment Options

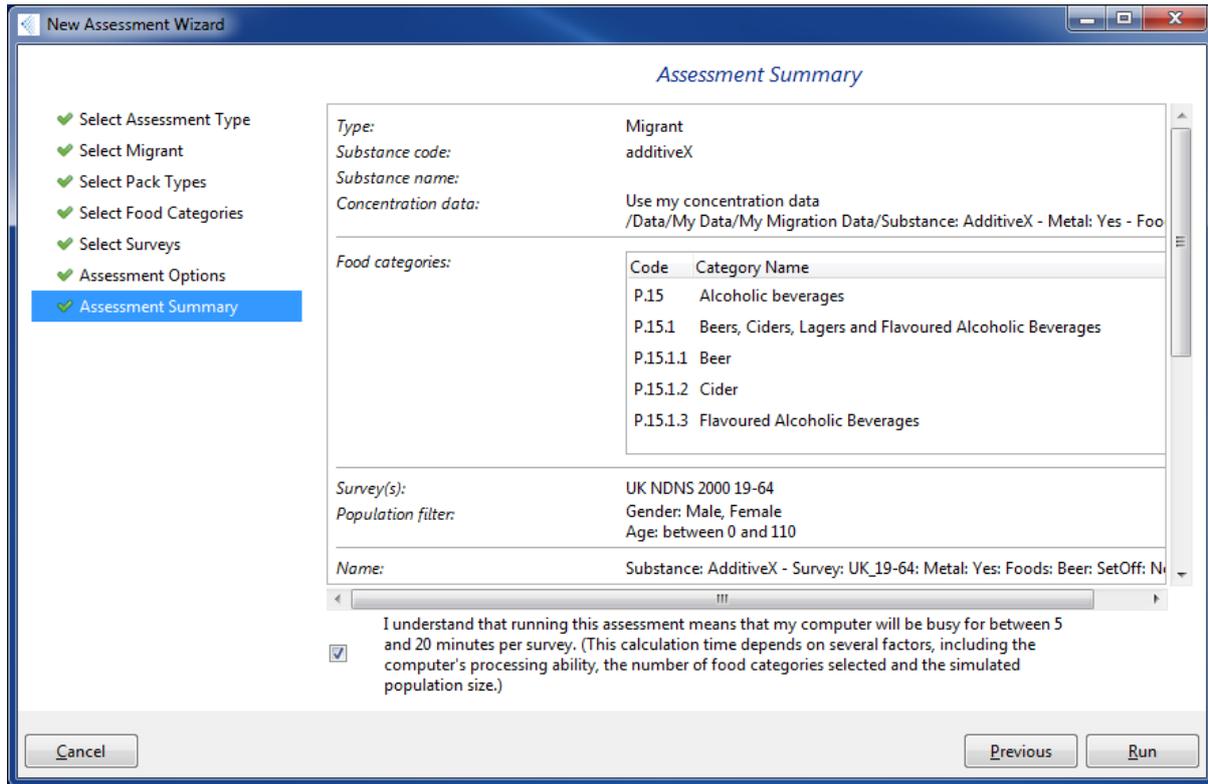


Figure 3-114: Assessment Summary

It is left up to the user to access the output of the resulting assessment (i.e. the assessment Substance: AdditiveX – Survey: UK\_19-64 - Metal: Yes - Foods: Beer - SetOff: No)

### 3.3.4 Exercises for Entering extraction/migration data

Use the “New Packaging Wizard” and “New Assessment” tools to initially establish the concentration levels of the given substance in the chosen foods in (i) and hence run an exposure assessment for the chosen country in (ii).

- (i) Existing Substance in Non-Metal Pack Type
  - a. Metal: No
  - b. Existing Substance: Yes
  - c. Substance: 1976 (ATBC)
  - d. Include set-off: No
  - e. Surface / Volume: 0.6
  - f. (Pack) Type: Flexible Wrapper /Bag/ Pouch
  - g. Material Code: M.9.2 OPP not voided
  - h. Concentration: 900
  - i. Thickness: 25
  - j. Food Categories: P.1.2.1 Processed Cheese
  - k. Pack Size: 1000.00
  - l. Time: 10 days
  - m. Temperature: 40 degrees centigrade

- n. Table Name: Substance: 1976 – Metal: No – SetOff: No – Food: Cheese
- (ii) Use the results in (i) to run a Packaging Assessment satisfying the following criteria:
  - a. Pack Types: All
  - b. Food Categories: P.1.2.1 Cheese
  - c. Survey: UK NDNS 2000 19-64
  - d. Assessment Name: Substance: 1976 – Metal: No – SetOff: No – Food: Cheese
  - e. Consumer Loyalty: Without
  - f. Use SetOff: No

### 3.4 Working at Lowest Tier

Earlier we ran the assessment “Substance: 1084 –Survey: UK\_19-64 – All Foods” as highlighted in Figure 3-115.

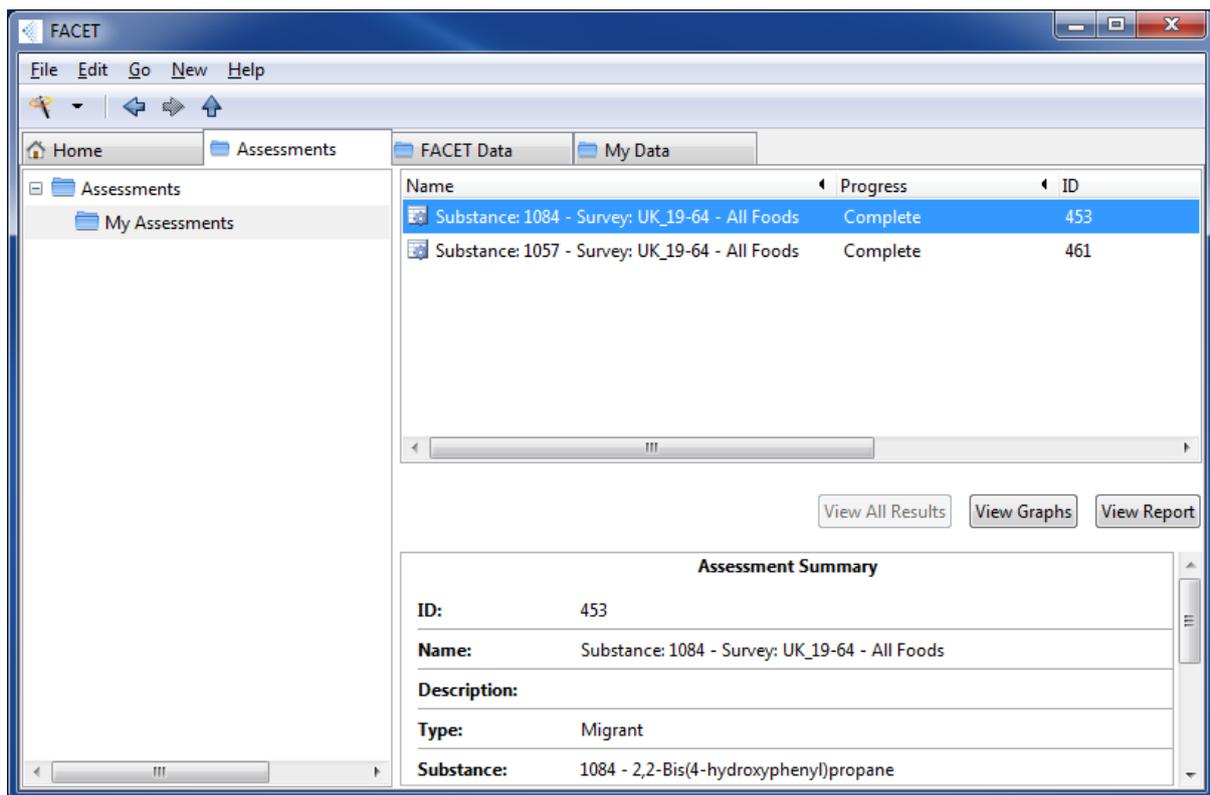


Figure 3-115: Already Run Assessment

Graphs relating to the outputs of the assessment are illustrated in Figure 3-116.

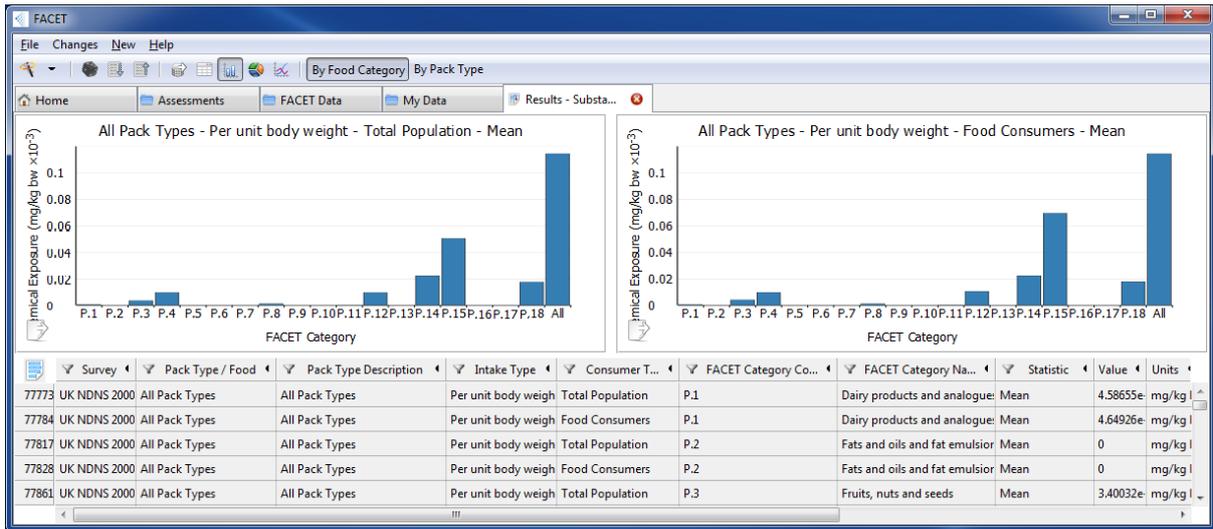


Figure 3-116: View Graphs

We observe that food categories P.15, P.14, P.18, P.12, P.4 are the main drivers, in that order. However no detail is provided at a lower tier. This means that when an assessment is run and “Include lowest tier results” is not selected, the exposure value for this food is described only for the parent food (e.g. P.15 Alcoholic Beverages) and not the foods at lower tiers (e.g. P.15.1.1 Beer, P.15.1.2 Cider, etc.). We have two options. The first is to repeat the assessment selecting the option at all tiers. This is time and memory intensive. The other option is identify the main drivers of the exposure and repeat the assessment at lower tiers for that food. An example of this is provided below where a lower tier assessment is run for P.15 (Alcoholic beverages). At this point the user follows the steps illustrated in Figure 3-117 to Figure 3-123.

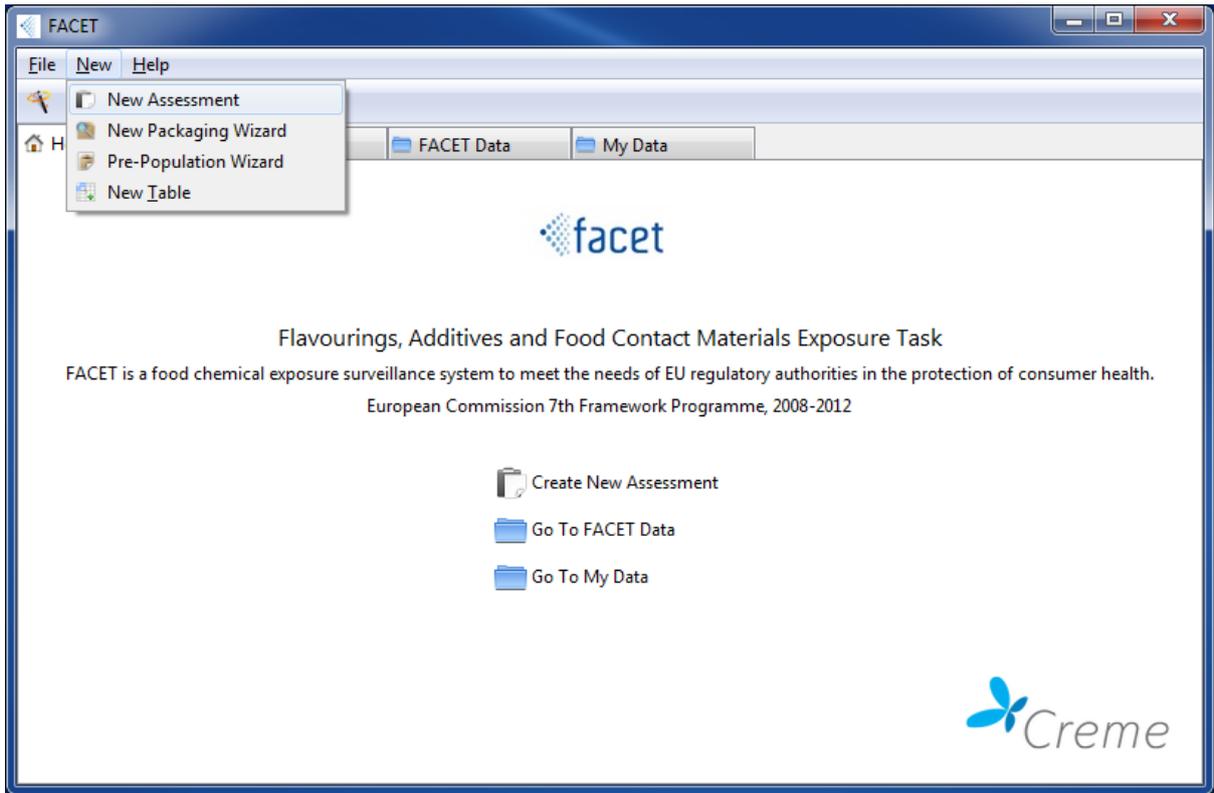


Figure 3-117: New Assessment

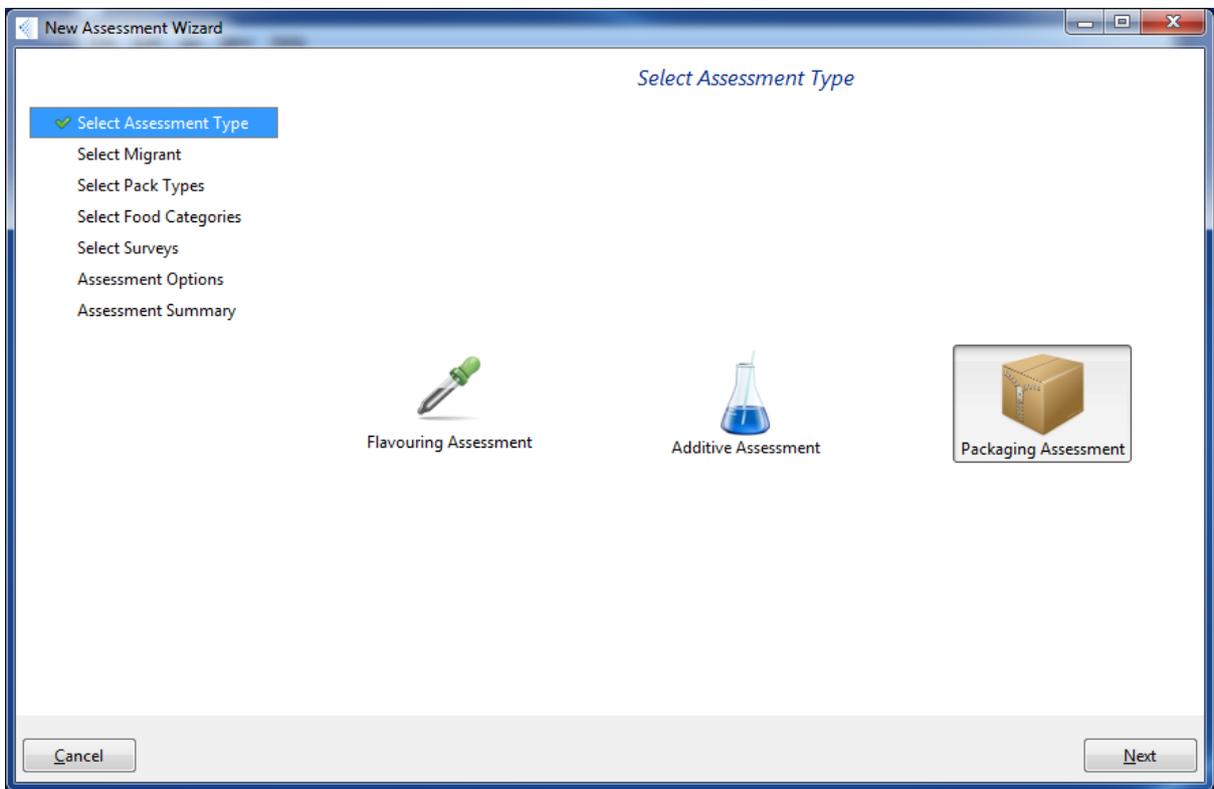


Figure 3-118: Packaging Assessment

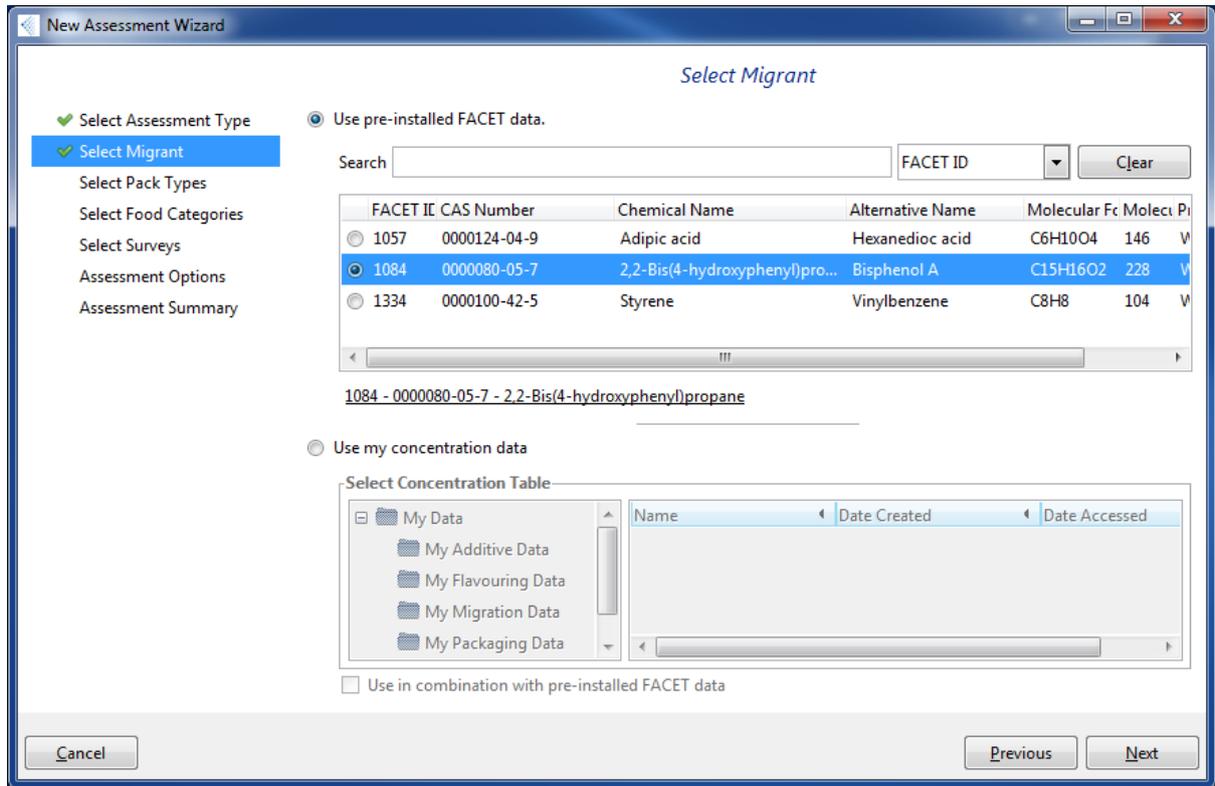


Figure 3-119: Select Migrant

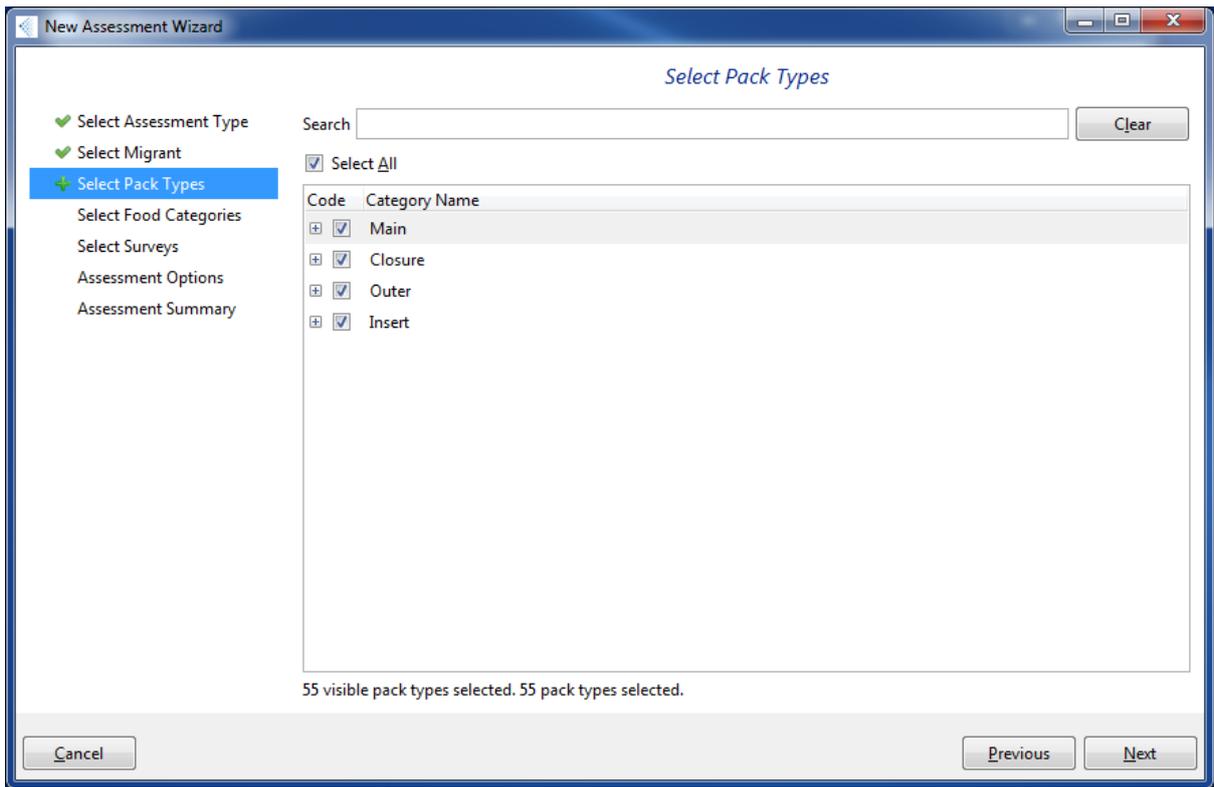


Figure 3-120: Select Pack Types

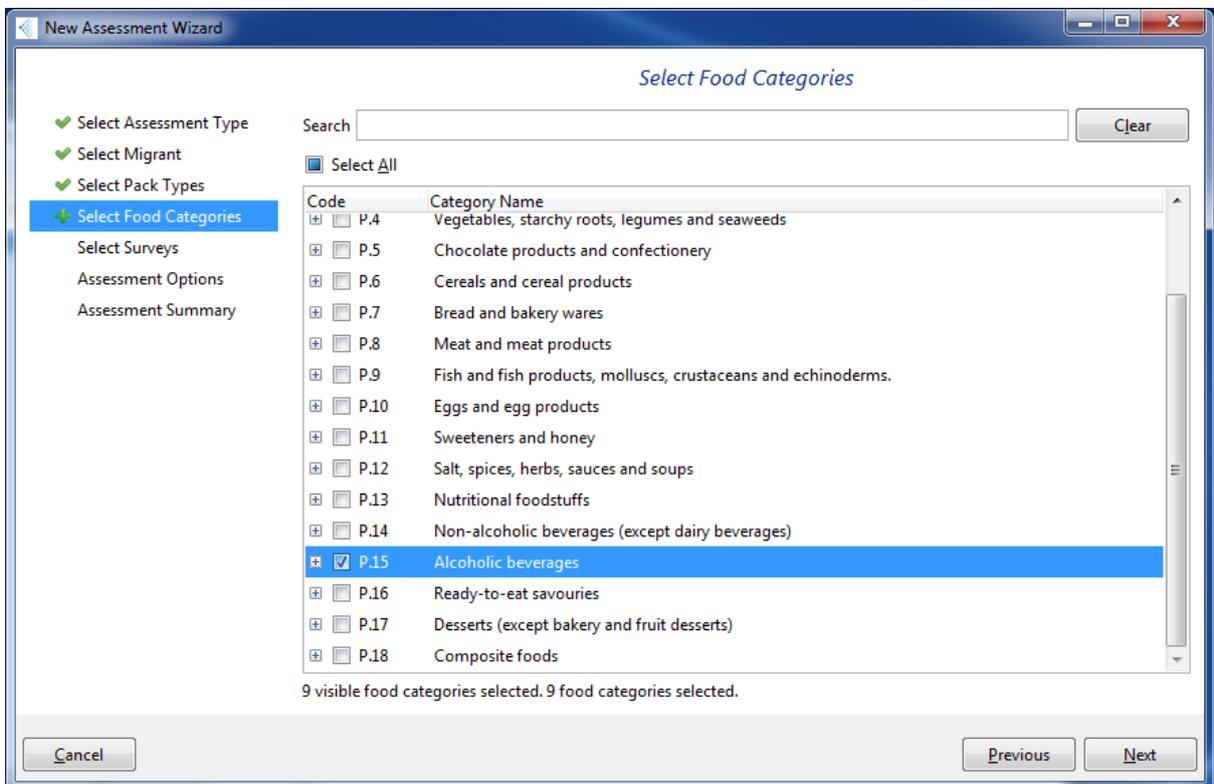


Figure 3-121: Select Food Categories

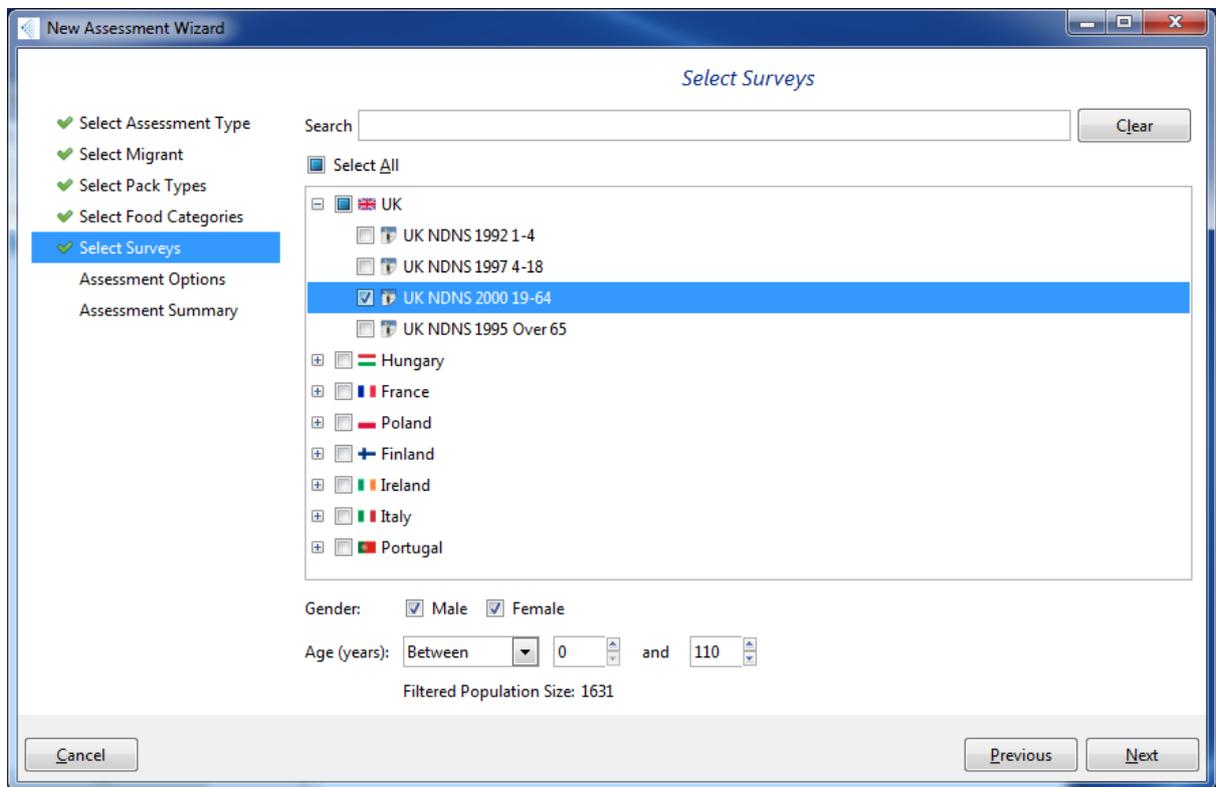


Figure 3-122: Select Survey

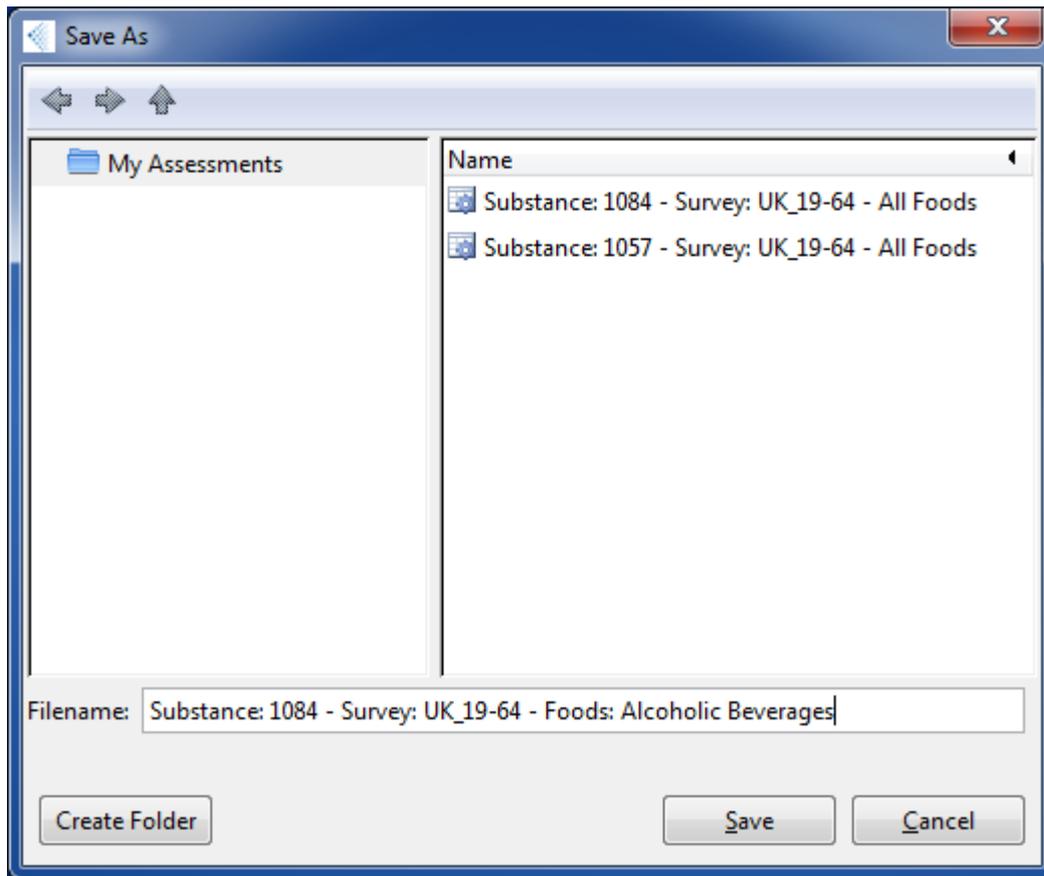


Figure 3-123: Naming Assessment

Now the user can access the “Assessment Options” and in particular the “Advanced Options”. In the “Advanced Options” the user should tick the “Include lowest tier results” option (as shown in Figure 3-124). This has the effect of providing exposure data for every food in the “P.15 Alcoholic Beverages” category. Without selecting this option, the software will calculate an exposure only at the highest tier (i.e. P.15 Alcoholic Beverages).

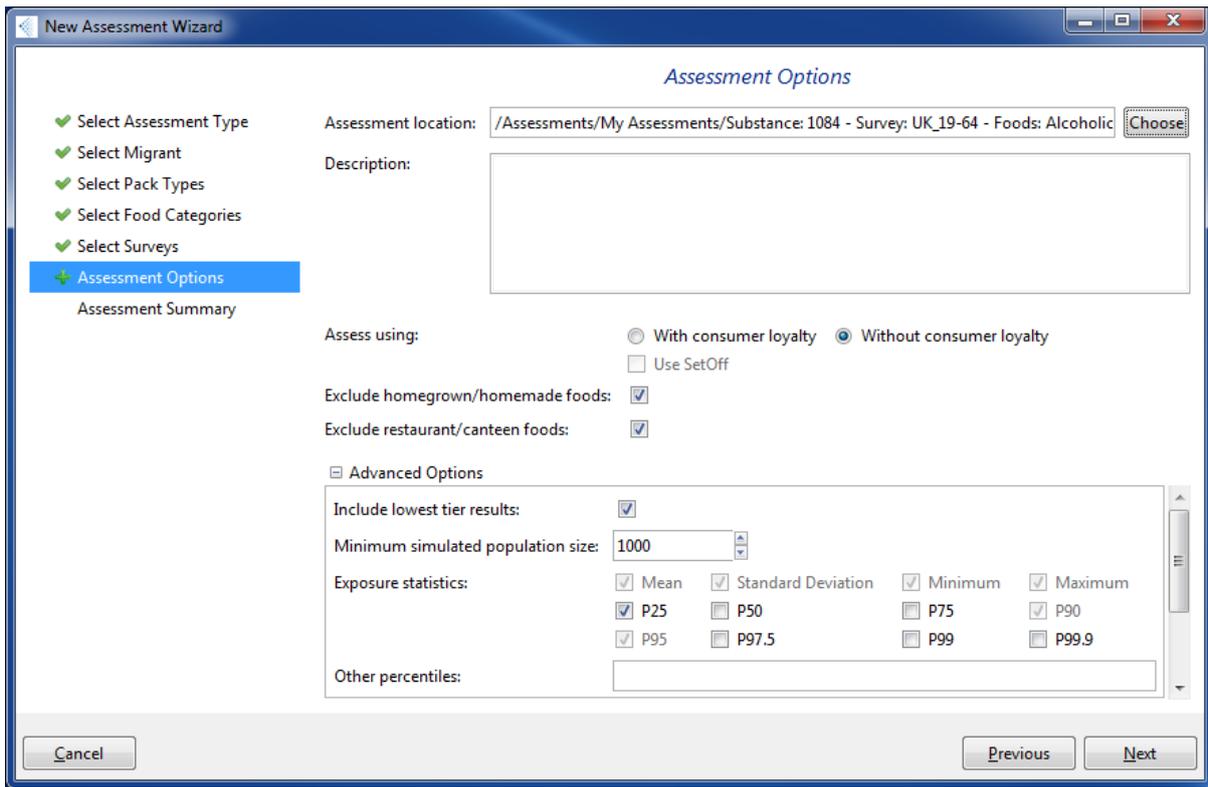


Figure 3-124: Selecting Lowest Tier Results

The assessment is now summarised and run as shown in Figure 3-125.

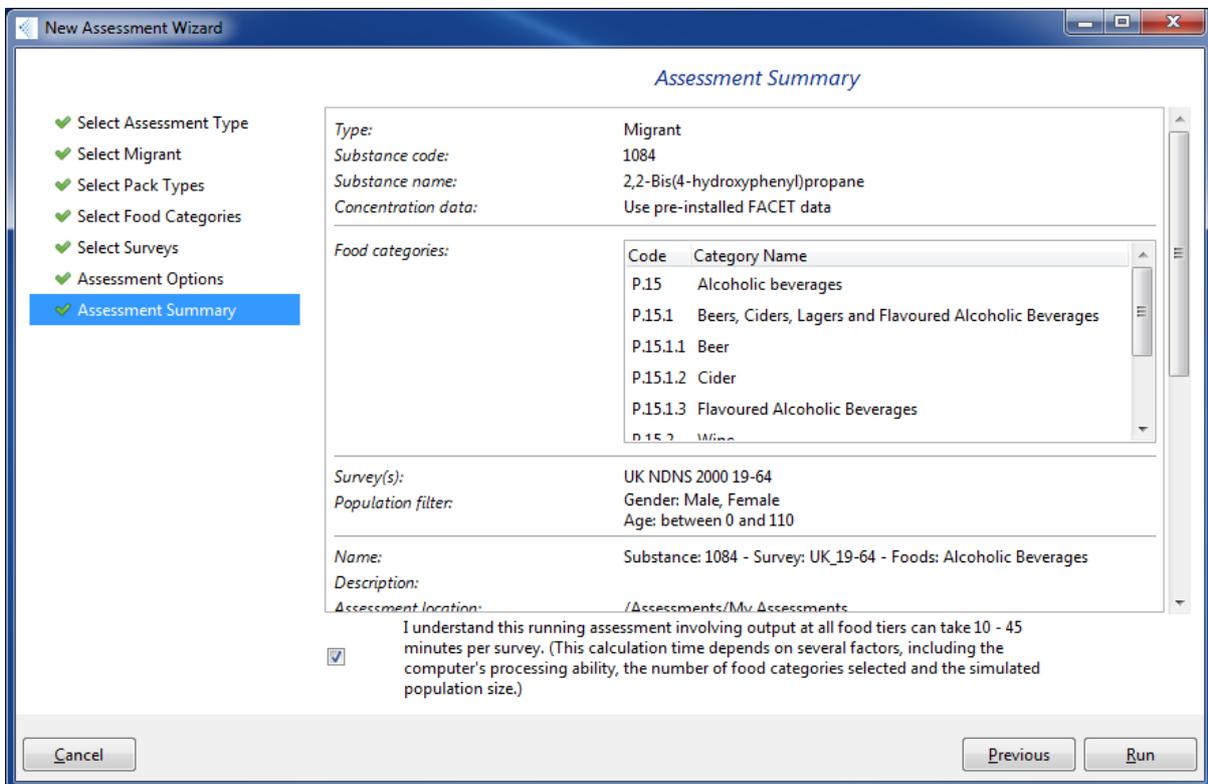


Figure 3-125: Assessment Summary

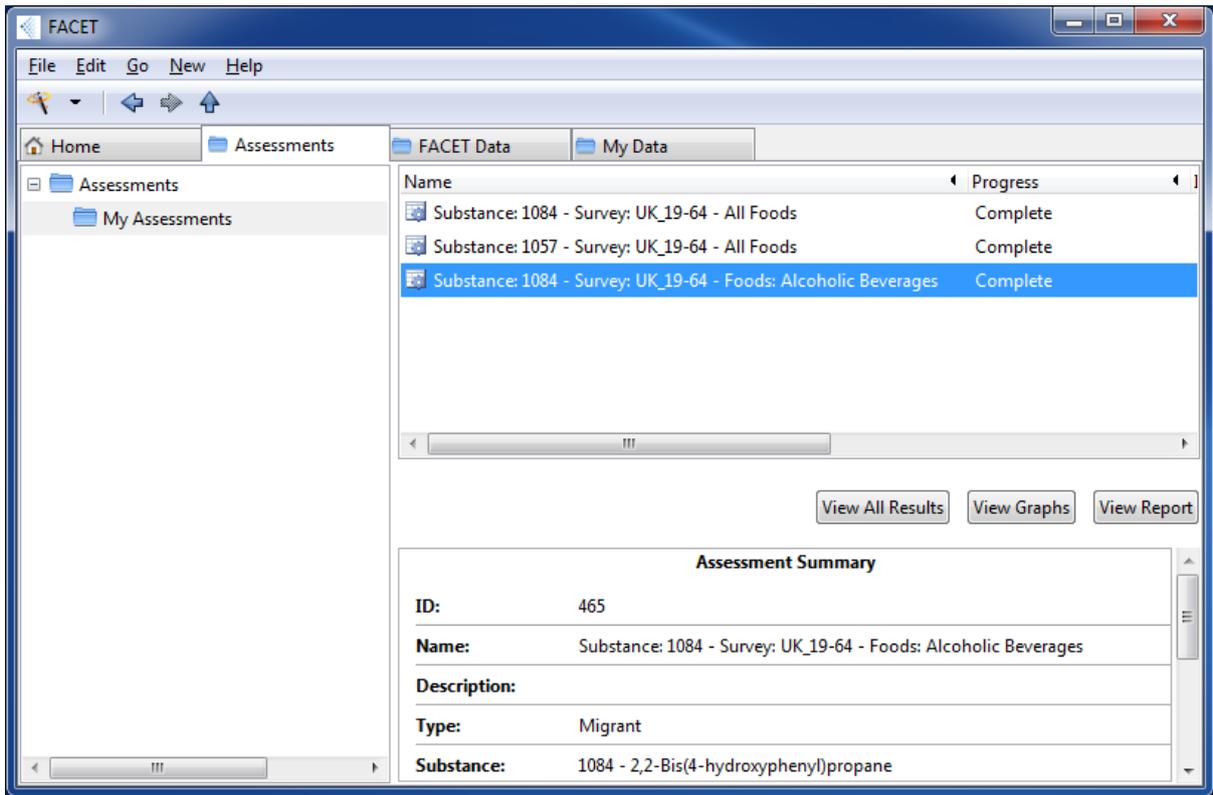


Figure 3-126: Assessment Complete

Following completion, the viewer has different options to view the results. If the user selects the “View All Results” option (shown in Figure 3-127 and Figure 3-128) then it is possible to view the results at the lowest tiers. However the “View Graphs” and “View Report” options still only provide exposure data at the higher tier (i.e. P15 Alcoholic Beverages in this example).

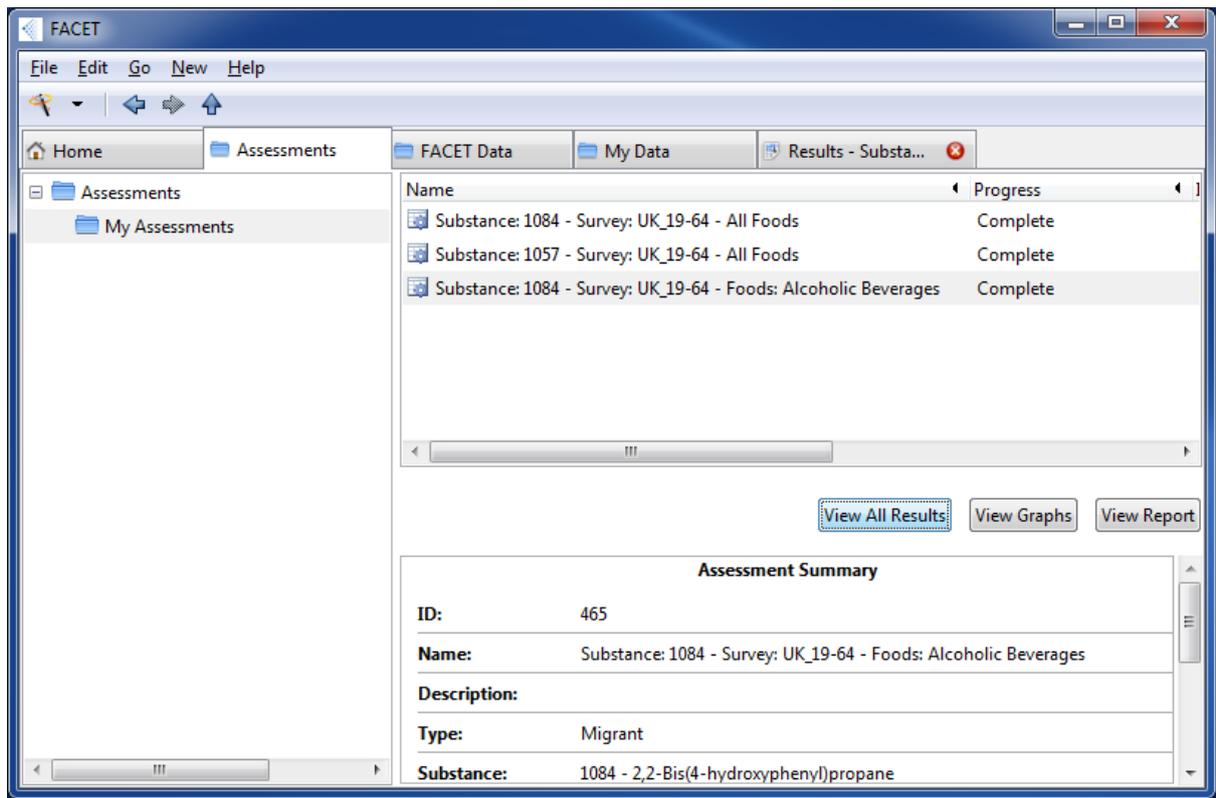


Figure 3-127: Select View Results to check at Lowest Tiers

	Consumer T...	FACET Food C...	FACET Food N...	Statistic	Value	Units	Standard Error	90'
20199	Population	P.15.3.1	Spirits	Mean	0	mg	0	
20221	Population	P.15.3.1	Spirits	Mean	0	mg/kg bw	0	
20243	Population	P.15.1.1	Beer	Mean	217.287	g	10.512	
20265	Population	P.15.1.1	Beer	Mean	2.77259	g/kg bw	0.13542	
20287	Population	P.15.1.2	Cider	Mean	19.7386	g	4.42073	
20309	Population	P.15.1.2	Cider	Mean	0.272662	g/kg bw	0.069255	
20331	Population	P.15.1.3	Flavoured Alcoholic Beve	Mean	9.95113	g	1.37345	
20353	Population	P.15.1.3	Flavoured Alcoholic Beve	Mean	0.13709	g/kg bw	0.0207831	
20375	Population	P.15.2.1	Wine	Mean	53.1079	g	2.6555	
20397	Population	P.15.2.1	Wine	Mean	0.721355	g/kg bw	0.0318761	
20419	Population	P.15.3.1	Spirits	Mean	6.03594	g	0.495681	
20441	Population	P.15.3.1	Spirits	Mean	0.0822354	g/kg bw	0.00642261	
20463	Population	P.15.1.1	Beer	Mean	0	mg	0	
20485	Population	P.15.1.1	Beer	Mean	0	mg/kg bw	0	
20507	Population	P.15.1.2	Cider	Mean	0	mq	0	

Figure 3-128: Examining Results

### 3.4.1 Exercises for Working at Lowest Tier

Exercises for Working at Lowest Tier

- (i) Run a Packaging Assessment (at the lowest tier) satisfying the following criteria
  - a. Substance: 1084
  - b. Pack Types: All
  - c. Food Categories: P.14 Non-alcoholic beverages
  - d. Survey: UK NDNS 2000 19-64
  - e. Loyalty: Without
  - f. Use SetOff: No

