

*DietaryBurdenCalculator*

A tutorial

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## 1 Overview

### 1.1 Introducing *DietaryBurdenCalculator*

- *DietaryBurdenCalculator* is based on a realistic dietary optimization scenario
- A flexible database is included in *DietaryBurdenCalculator*
- It is simple to use
- *DietaryBurdenCalculator* represents a fully transparent process

### 1.2 Installing *DietaryBurdenCalculator*

Open Setup File and follow further instructions (see Annex II).

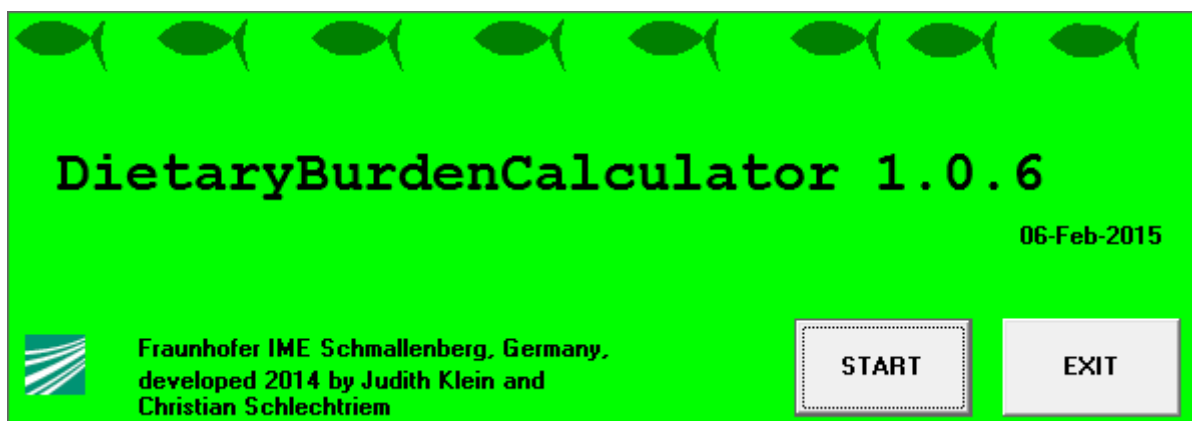
## 2 Introduction

The uptake of pesticides by fish and their resulting presence in fish products can occur following the ingestion of feed containing a pesticide residue. It is therefore necessary to evaluate residues in products of fish origin (EU Directive EC 1107/2009). Fish metabolism data can determine total residue levels and the chemical nature of residues in the edible tissues of fish exposed to pesticides. According to the working document on the Nature of Residues in Fish (European Commission, 2013), fish metabolism studies are required when pesticide use may lead to significant residues in fish feed, generally considered to be  $\geq 0.1$  mg/kg of the total diet. Fish in intensive aquaculture production systems are fed according to a maximum reasonably balanced diet (MRBD) approach. Therefore, the maximum dietary burden of a pesticide in fish feed needs to be calculated based on the formulation of MRBD, taking into account the specific residue values in all feedstuffs, based on supervised trials where available. The procedure described in the working document can only provide an approximation of the dietary burden in aquaculture diets. In practice, the MRBD should be calculated by linear programming to optimize the dietary burden estimates.

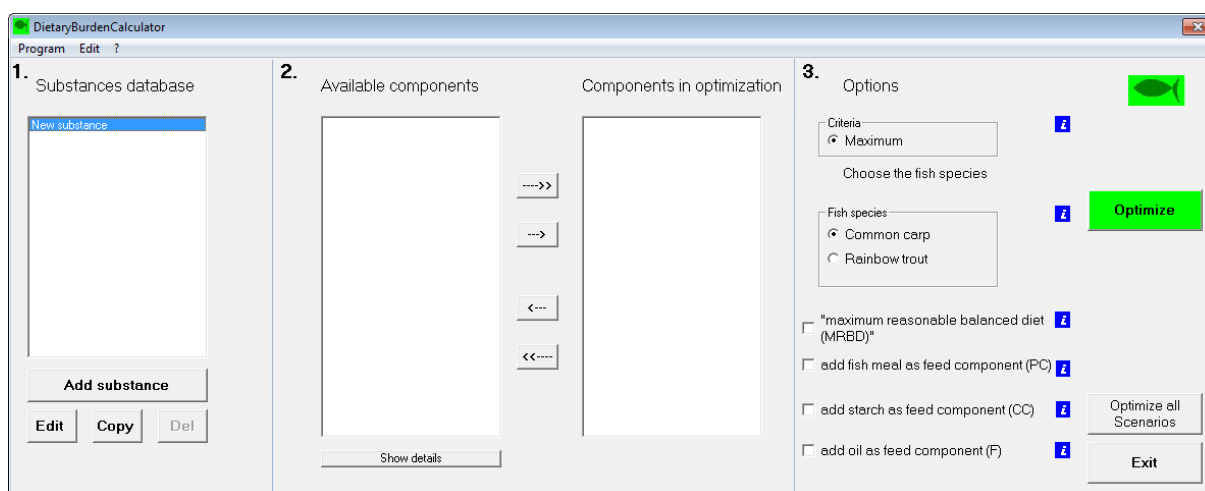
## 3 Working with DietaryBurdenCalculator

### 3.1 Start *DietaryBurdenCalculator*


After installing and starting *DietaryBurdenCalculator*, you will see the startup window. For continuing the program press "START".



You will now see the graphical user interface which is divided into three sections: The substances database (1), components (2) and optimization options (3). We will work our way from the left to the right.



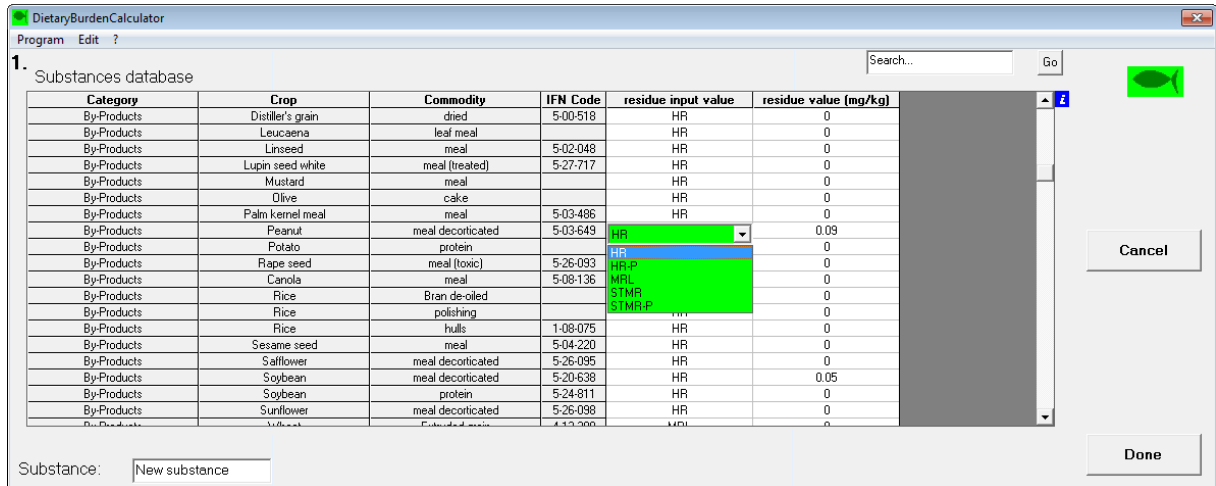
### 3.2 Obtaining help

To bring up the help menu, press the help tab or F1 on your keyboard. The help menu opens in a separate window. Further information can also be obtained by pressing .

### 3.3 Substances database

In the left section, the substances database (1) can be found. Customize the substances database by following these steps.

To	Do this
Add substances.	Click on "Add substance" to bring up the database window.
Edit residue values for selected substances.	Click on "Edit" to bring up the database window and enter residue values.
Copy a substance including all its entries.	Click on "Copy" and the copied substance appears at the end of the list.
Delete a substance from the list.	Click on a substance to select it. Then press "Del".



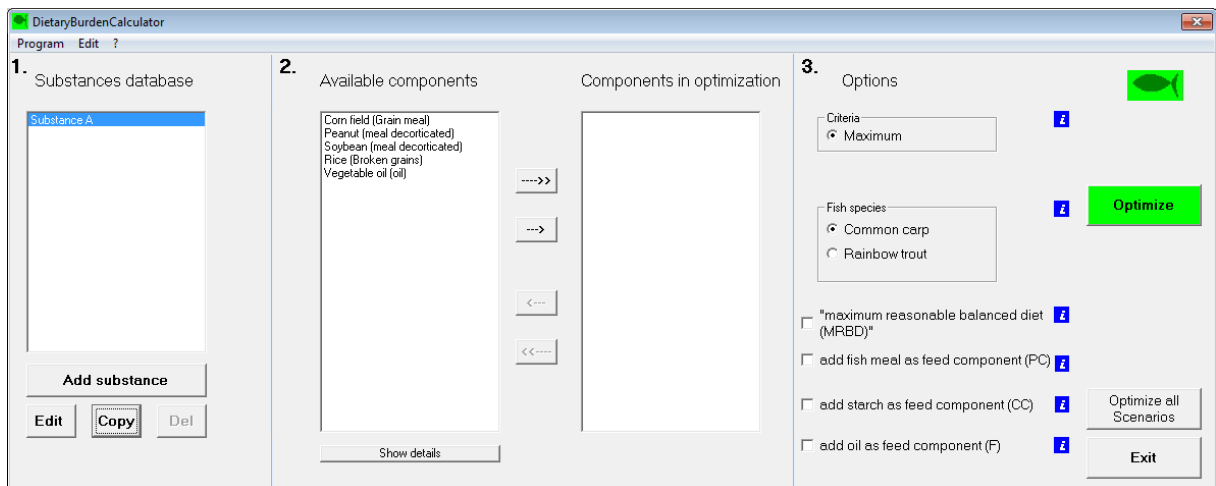
The substances database window offers the possibility to enter different classes of residue values (HR, HR-P, MRL, STMR, STMR-P). The residue values (mg/kg) are inserted in the right column.

To	Do this
Change class of residue value	Select a residue value class from the drop down menu.
Change residue value.	Enter residue value and press enter.





To return to the user interface, press "Done" (after modifying a value class or value).

### 3.4 Select components

The middle section (2) is divided into two boxes: "Available components" and "Components in optimization". The "Available components" box contains all components with a residue value greater than zero (based on entries in substances database) for the selected substance.

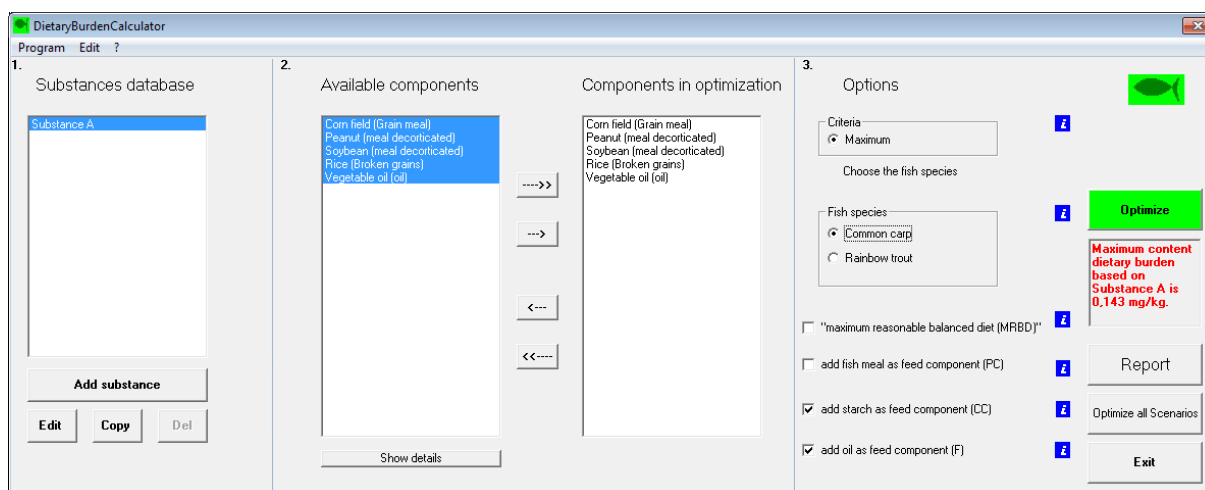


You can choose single or multiple components for optimization by following these steps.

To	Do this
Get more information on the available components.	Press the "Show details" button.
Select all available components for optimization.	Press  .
Select individual components from the list of available components.	Select the desired component for optimization. Press  . Repeat for each component that you want to choose for optimization.
Remove all selected components from optimization list.	Press  .
Remove individual components from the list of components selected for optimization.	Select the desired component from the optimization list and press  .

### 3.5 Optimization

The "Options" section on the right (3) gives you different possibilities to calculate the maximum dietary burden.

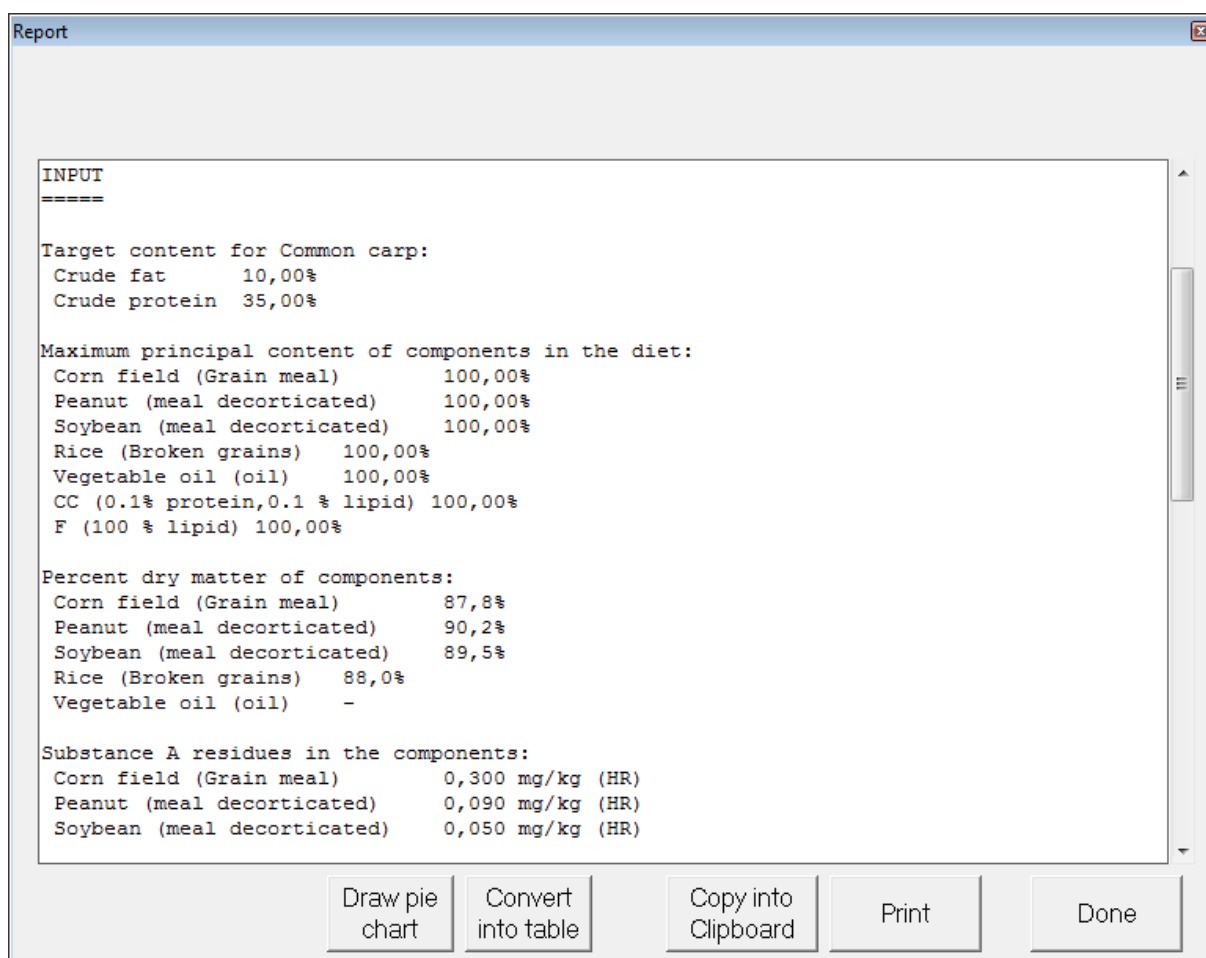


To	Do this
Select a fish species for which optimization should be conducted.	Select between common carp and rainbow trout. Press "Optimize".
Consider the maximum reasonable balanced diet (MRBD) in optimization (See Chapter 3.7).	Select "Maximum reasonable balanced diet". Press "Optimize".
Add protein concentrate (PC) as additional feed component (uncontaminated).	Select "Add fish meal as feed component (PC)". Press "Optimize".
Add carbohydrate concentrate (CC) as additional feed component (uncontaminated).	Select "Add starch as feed component (CC)". Press "Optimize".
Add fat (F) as additional feed component (uncontaminated).	Select "Add oil as feed component (F)". Press "Optimize".
Include all possible scenarios in optimization.	Select a fish species and press the "Optimize all scenarios" button.

Inclusion of additional feed components (uncontaminated) might be necessary in case the available/ selected components cannot be mixed in a way to reach the target composition of the test diet (depending on fish species) (See Chapter 4).

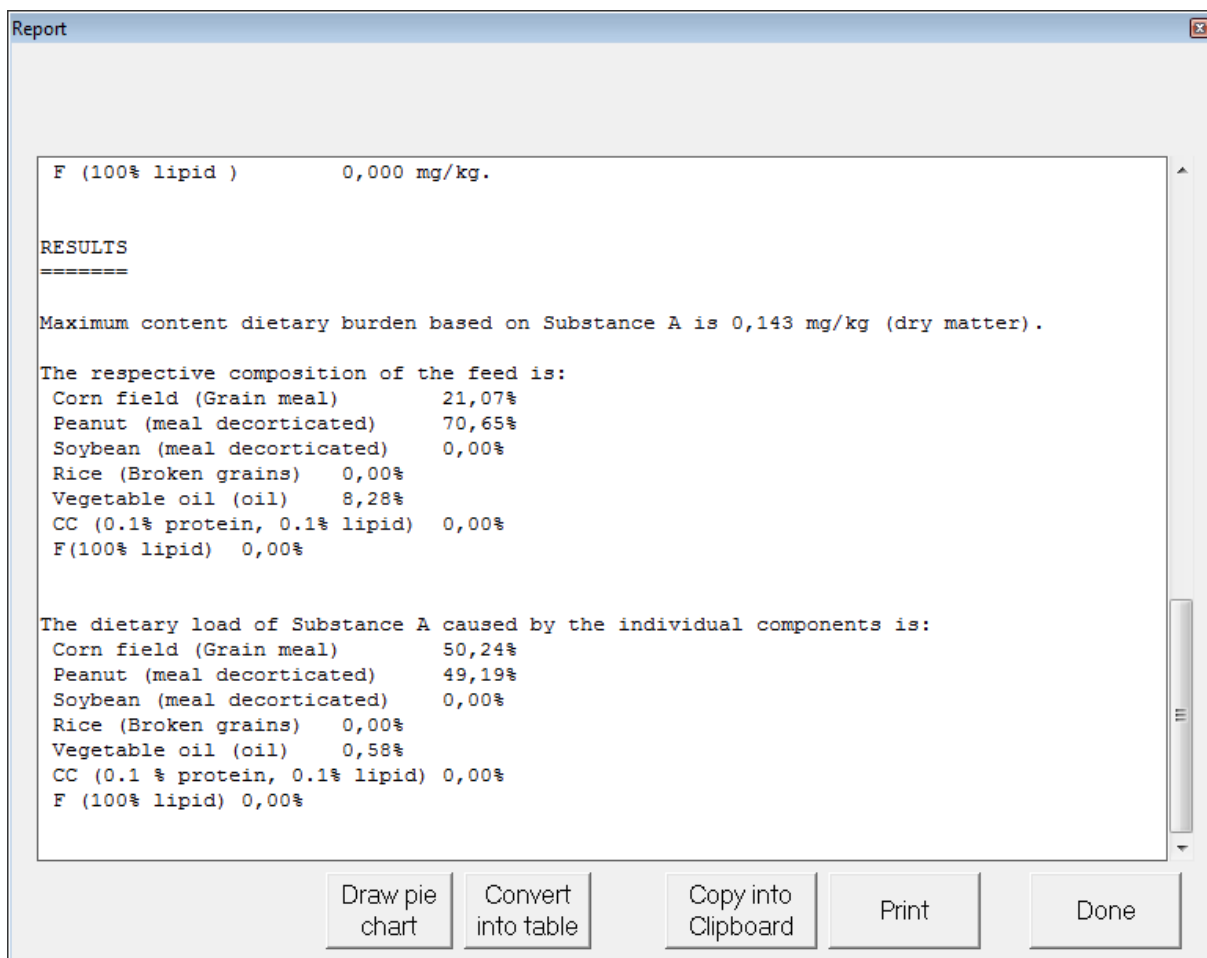
### 3.6 Output

Below the “Optimize” button, the calculated maximum dietary burden (in mg/kg) appears in a box. By clicking on the “Report” button, the report opens. It is divided into two sections, input and report.



Input:

Paragraph	Gives you information on	Can be modified by
Target content for selected fish species.	Target composition of test diet (% dry matter) of selected fish species	Choosing other fish species in optimization options.
Maximum principal content of components in the diet.	The maximum possible inclusion rate (%; no restrictions applied) of selected components in diet.	Selecting maximum reasonable balanced diet (MRBD) in optimization options (see Chapter 3.7).
Percent dry matter of components.	Dry matter content of each selected commodity.	-
Substance residues in the components.	Substance residues in each selected commodity.	-
Substance residues in the components.	Substance residues (dry matter) in each selected commodity.	-



Results:

Paragraph	Gives you information on
Maximum content dietary burden.	Result of dietary burden calculation.
Respective composition of the feed.	Feed composition leading to the maximum dietary burden.
Dietary load of substance caused by individual components.	Percent contribution of each commodity to maximum dietary burden.

To proceed, the following options are available.

To	Do this
Create a pie chart.	Click on "Draw pie chart".
Create a table.	Click on "Convert into table".
Copy results into clipboard.	Click on the "Copy into Clipboard" button.
Print the results.	Click on the "Print" button.
Close the report.	Press the "Done" button.



“Optimize all scenarios” gives you the following report:

Report

Substance: **Substance A**      Species: **Common carp (10,00% Lipid; 35,00% Protein)**

Szenario	Description	Maximum Residue Value	
1	Without PC, CC, F	0,143	Details
2	Without PC, CC, F - "maximum reasonable balanced diet (MRBD)"	0,136	Details
3	PC	0,190	Details
4	PC - "maximum reasonable balanced diet (MRBD)"	0,160	Details
5	CC used	0,143	Details
6	CC used with - "maximum reasonable balanced diet (MRBD)"	0,136	Details
7	F used	0,143	Details
8	F used with - "maximum reasonable balanced diet (MRBD)"	0,136	Details
9	PC and CC used	0,190	Details
10	PC and CC used - "maximum reasonable balanced diet (MRBD)"	0,160	Details
11	PC and F used	0,190	Details
12	PC and F used - "maximum reasonable balanced diet (MRBD)"	0,160	Details
13	CC and F used	0,143	Details
14	CC and F used - "maximum reasonable balanced diet (MRBD)"	0,136	Details
15	PC, CC and F used	0,190	Details
16	PC, CC and F used - "maximum reasonable balanced diet (MRBD)"	0,160	Details

Open Full Report File      Copy into Clipboard      Print      Done

By clicking on the “Details” button, a report as previously described can be produced for each of the 16 scenarios. All scenarios are summarized in one report by clicking on “Open Full Report File”.

The scenarios cover all possible combinations including addition of uncontaminated feed components (PC, CC, F) and the consideration of maximum inclusion rates for selected commodities (MRBD; see Chapter 3.7).

The following scenarios are available:

<b>Scenario</b>	<b>Explanation</b>
1	Without PC, CC; F (only selected commodities)
2	Without PC, CC; F – maximum reasonable balanced diet (MRBD) with selected commodities
3	Selected commodities plus uncontaminated fish meal (PC) with 75% protein, 5% lipid
4	Selected commodities plus fish meal (PC) - maximum reasonable balanced diet (MRBD)
5	Selected commodities plus uncontaminated starch (CC)
6	Selected commodities plus CC - maximum reasonable balanced diet (MRBD)
7	Selected commodities plus uncontaminated oil (F)
8	Selected commodities plus F - maximum reasonable balanced diet (MRBD)
9	Selected commodities plus fish meal and CC
10	Selected commodities plus fish meal and CC - maximum reasonable balanced diet (MRBD)
11	Selected commodities plus fish meal and F
12	Selected commodities plus fish meal and F - maximum reasonable balanced diet (MRBD)
13	Selected commodities plus CC and F
14	Selected commodities plus CC and F - maximum reasonable balanced diet (MRBD)
15	Selected commodities plus fish meal, CC and F
16	Selected commodities plus fish meal, CC and F - maximum reasonable balanced diet (MRBD)

### 3.7 Consider maximum reasonable balanced diet (MRBD)

To open the list of feed components, pull down the "Edit" menu and select "Feed components". The list of feed components opens.

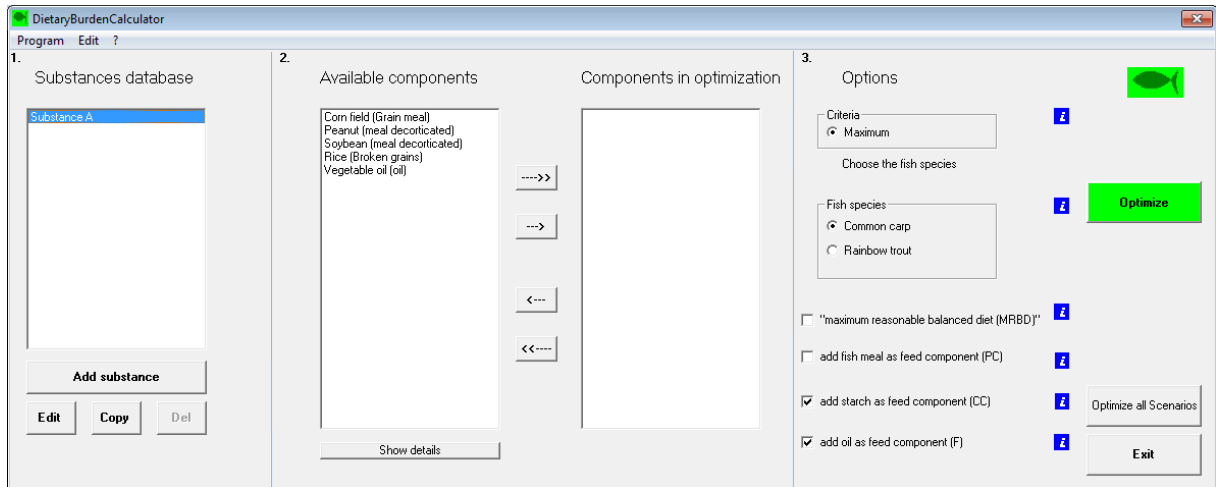
Crop	Commodity	IFN Code	CP[%] of DM	CL[%] of DM	DM[%]	Carp (max % of diet)	Trout (max % of diet)
Barley	bran fractions	4-00-515	16,4	66	88	35	15
Brewer's grain	dried	5-00-516	25,9	7	92	35	15
Coconut/Copra	meal decorticated	5-01-572	44,2	1,2	91	25	15
Corn field	Grain meal	4-12-208	10,2	4,8	87,8	35	20
Corn field	bran	5-28-235	15	5,7	87,5	20	5
Corn field	hominy meal	4-03-010	8,9	5,4	90,1	35	20
Corn gluten	feed	5-28-243	24,7	3,5	90,1	20	10
Corn gluten	meal	5-28-242	59,9	3,6	91,3	20	15
Corn	starch	4-02-889	0,4	0,4	90,2	35	15
Cottonseed	meal	5-01-617	32,9	1,7	90	35	15
Distiller's grain	dried	5-00-518	28,5	10,2	92	10	10
Leucaena	leaf meal		24,5	5,4	90,5	10	100
Linseed	meal	5-02-048	35	2	90	35	15
Lupin seed white	meal (treated)	5-27-717	34,5	6,1	89,5	15	15
Mustard	meal		42,4	1,8	89,9	10	10
Olive	cake		13,3	3,6	92,4	10	10
Palm kernel meal	meal	5-03-486	16,3	1,4	90	10	8
Peanut	meal decorticated	5-03-649	46,5	1	90,2	35	15
Potato	protein		81,8	2,8	89,4	3	100
Rape seed	meal (toxic)	5-26-093	37,3	1,9	91	5	5
Canola	meal	5-08-136	37,3	1,9	91	35	20
Rice	Bran de-oiled		15,1	1,7	100	35	15
Rice	polishing		13,6	14,5	100	50	10
Rice	hulls	1-08-075	3,1	1	100	5	0
Sesame seed	meal	5-04-220	45	4,8	92,4	35	15
Safflower	meal decorticated	5-26-095	45,2	6,9	91	7	7
Soybean	meal decorticated	5-20-638	49,8	0,8	89,5	40	25
Soybean	protein	5-24-811	72	1	92	20	20

The table contains information on the protein content (CP, % of dry matter), lipid content (CL, % of dry matter) and dry matter (%) of each plant derived feed commodity. The last two columns contain maximum inclusion rates for the commodities used in carp and trout diets. By selecting maximum reasonable balanced diet (MRBD), the limits of selected commodities listed here are considered.

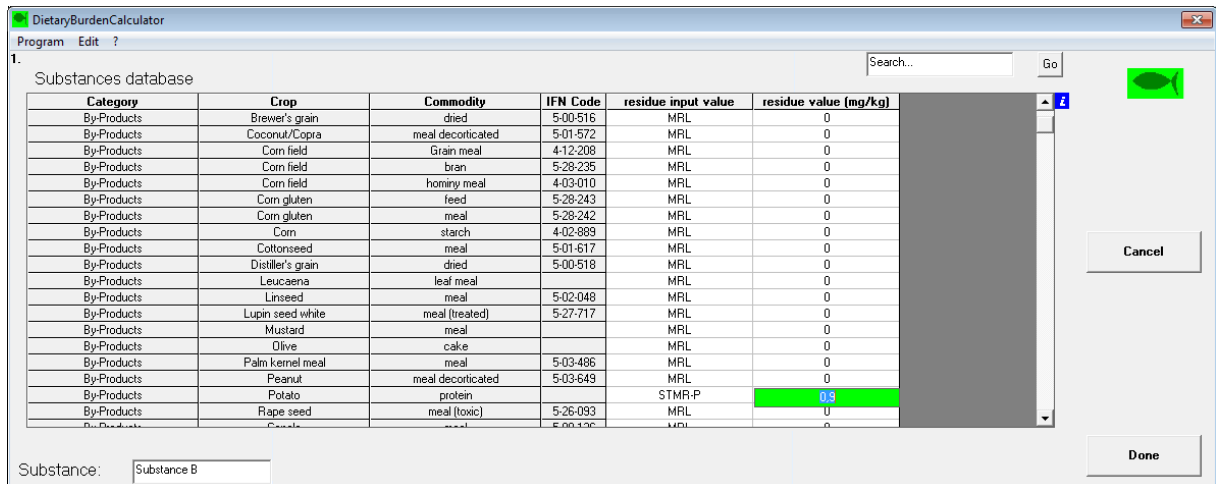
To	Do this
Delete a record.	Click on "Del Record".
Add a new record.	Click on "New Record".
Print the list of feed components.	Click on "Print".
Copy the list to clipboard.	Click on "Copy to Clipboard".
Save changes.	Press "Save".

## 4 Example

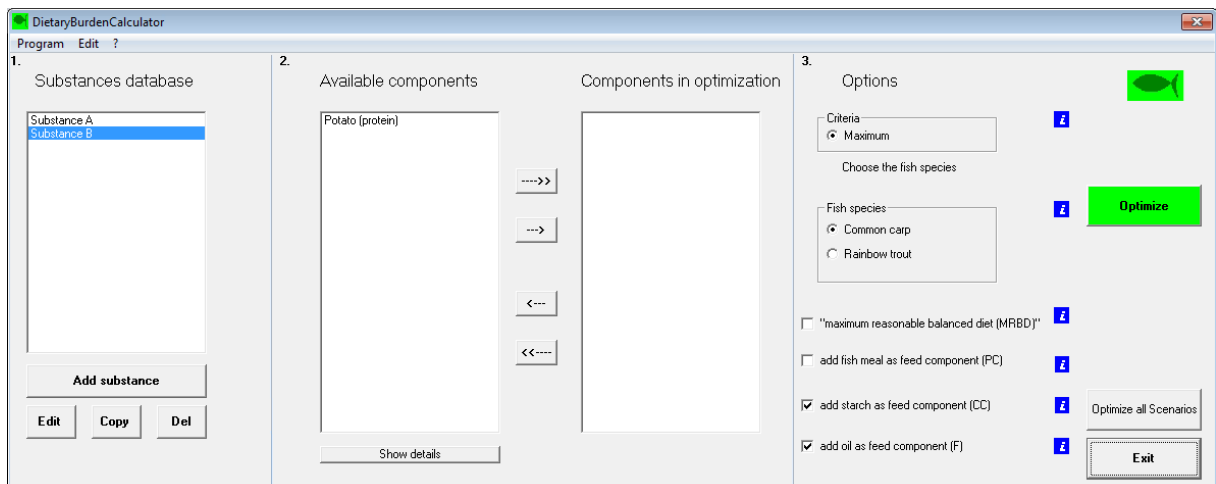
A new substance (Substance B) is added to the substances database by pressing "Add substance".



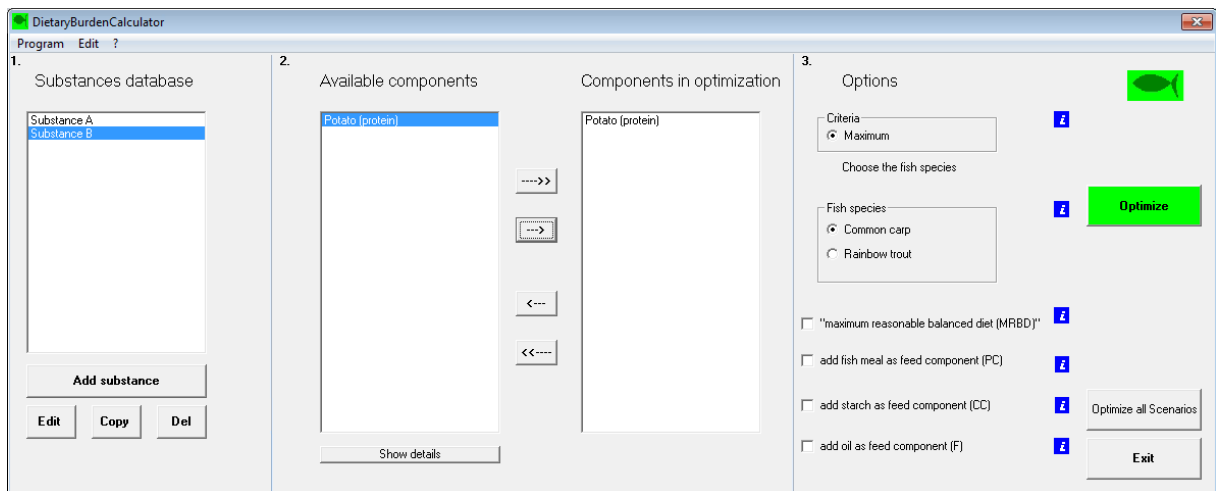
In the substances database, a STMR-P value of 0.9 mg/kg is inserted for potato protein. Then the database is closed by pressing "Done".



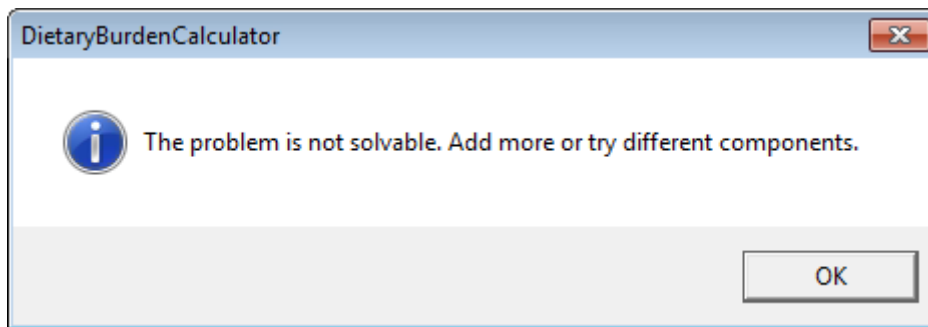
Now, the new substance (Substance B) is listed and only one component with a residue value higher than zero (potato protein) is available.



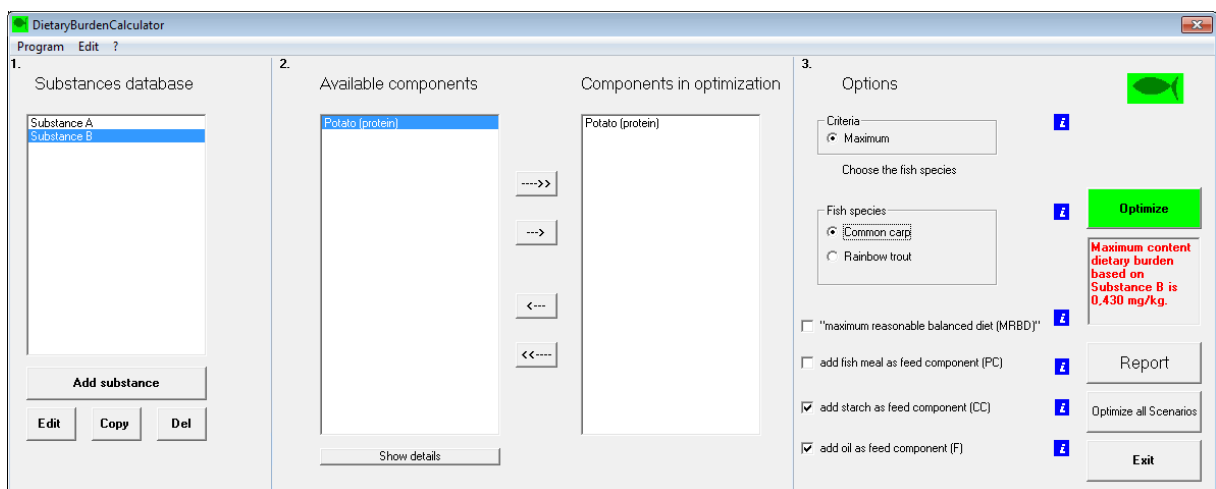
Potato protein is selected for optimization and the "Optimize" button is pressed.



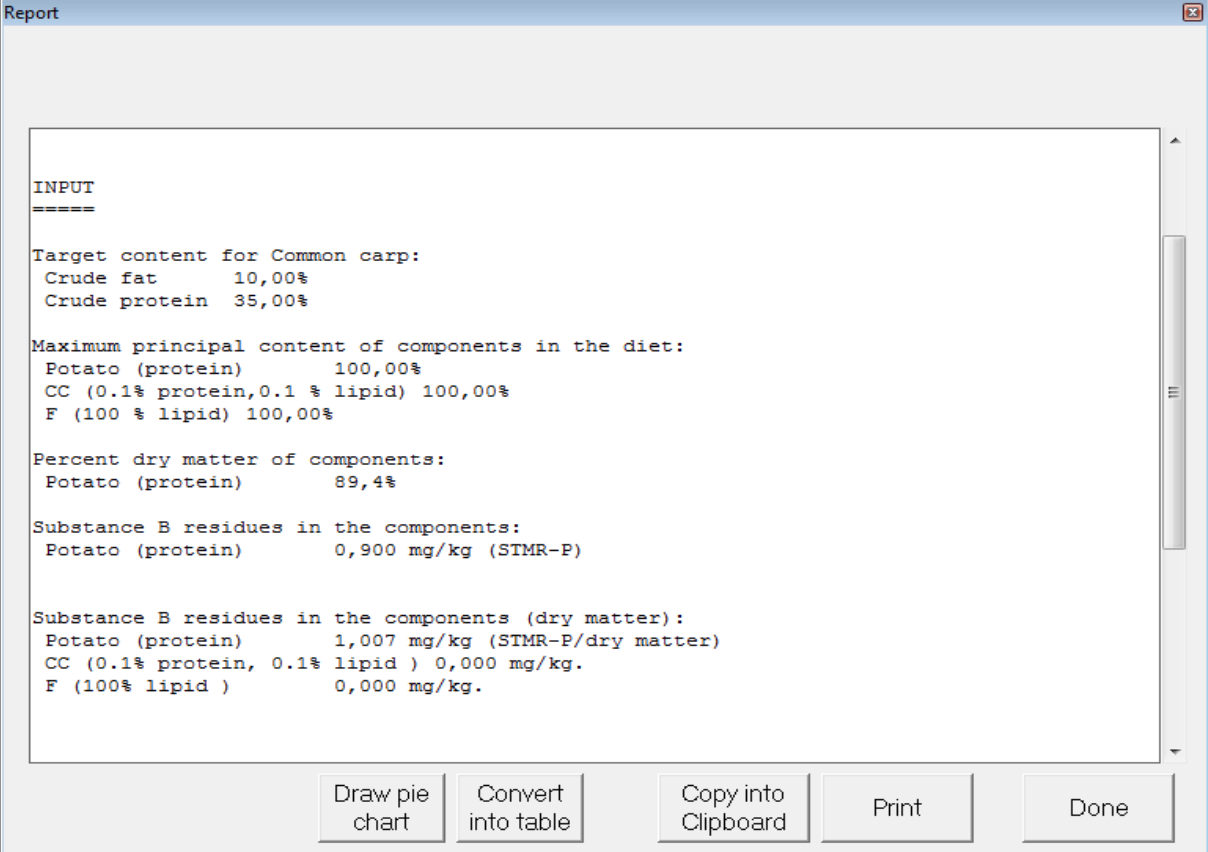
A new window opens with the following comment:



In the optimization options, additional uncontaminated components have to be added to the diet otherwise no maximum dietary burden can be calculated. Because protein is sufficiently provided by potato protein as single component, starch and oil have to be added to the diet to reach the target composition for the selected fish species. Now a maximum burden of pesticide residues can be determined.



By pressing the "Report" button, input and results can be viewed.



The screenshot shows a window titled "Report" with a text area containing the following input data:

```
INPUT
=====

Target content for Common carp:
Crude fat      10,00%
Crude protein  35,00%

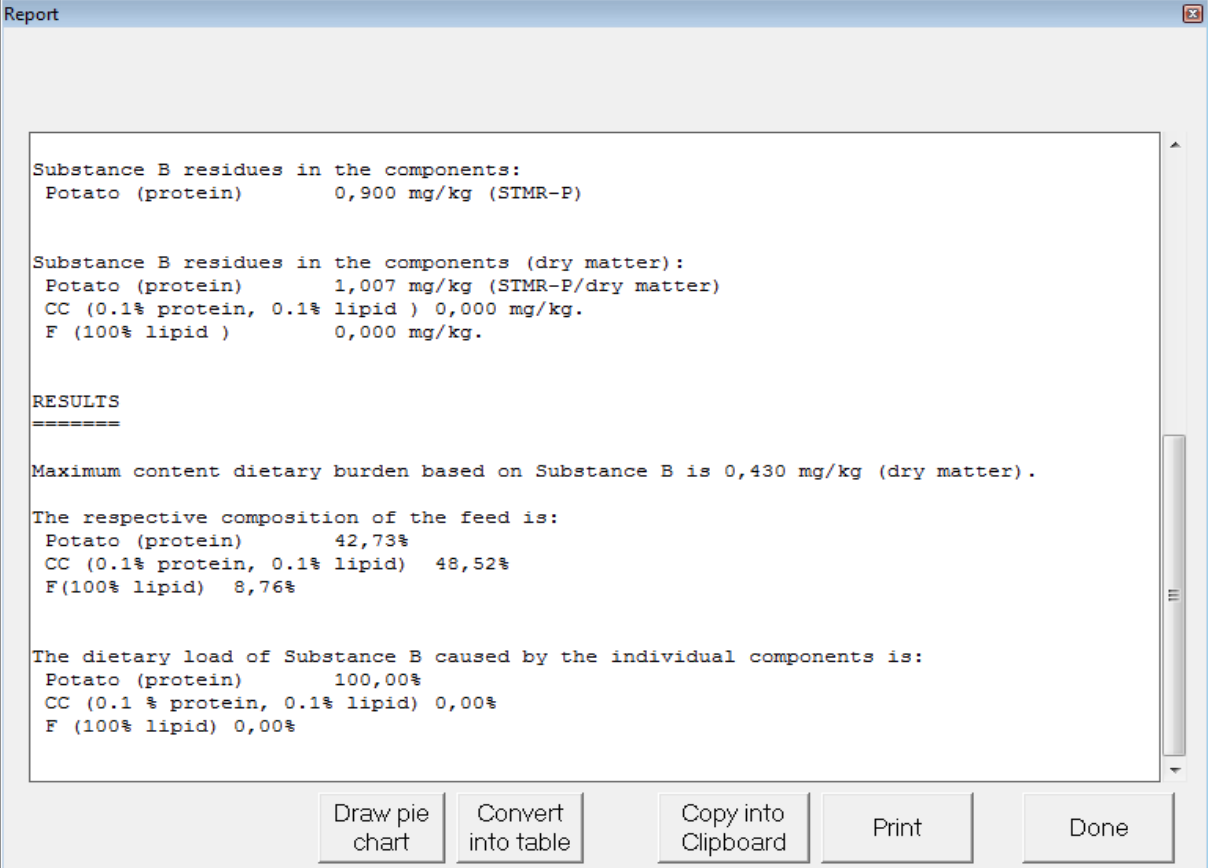
Maximum principal content of components in the diet:
Potato (protein)      100,00%
CC (0.1% protein,0.1 % lipid) 100,00%
F (100 % lipid) 100,00%

Percent dry matter of components:
Potato (protein)      89,4%

Substance B residues in the components:
Potato (protein)      0,900 mg/kg (STMR-P)

Substance B residues in the components (dry matter):
Potato (protein)      1,007 mg/kg (STMR-P/dry matter)
CC (0.1% protein, 0.1% lipid ) 0,000 mg/kg.
F (100% lipid )      0,000 mg/kg.
```

At the bottom of the window, there are five buttons: "Draw pie chart", "Convert into table", "Copy into Clipboard", "Print", and "Done".



The screenshot shows the same "Report" window, but now displaying the results of the calculation:

```
Substance B residues in the components:
Potato (protein)      0,900 mg/kg (STMR-P)

Substance B residues in the components (dry matter):
Potato (protein)      1,007 mg/kg (STMR-P/dry matter)
CC (0.1% protein, 0.1% lipid ) 0,000 mg/kg.
F (100% lipid )      0,000 mg/kg.

RESULTS
=====

Maximum content dietary burden based on Substance B is 0,430 mg/kg (dry matter).

The respective composition of the feed is:
Potato (protein)      42,73%
CC (0.1% protein, 0.1% lipid) 48,52%
F(100% lipid) 8,76%

The dietary load of Substance B caused by the individual components is:
Potato (protein)      100,00%
CC (0.1 % protein, 0.1% lipid) 0,00%
F (100% lipid) 0,00%
```

The same five buttons are present at the bottom: "Draw pie chart", "Convert into table", "Copy into Clipboard", "Print", and "Done".

## **5 References**

- [1] European Union, Regulation (EC) No 1107009 of the European Parliament and of the Council of 21 October 2009 concerning the placing of plant protection products on the market and repealing Council Directives 79/117/EEC and 91/414/EEC. OJ L309, 24.11.2009, pp. 1 – 50 (2009).
- [2] European Commission, Working document on 'Nature of Residues in Fish' SANCO/11187/2013 rev.3, 31 January 2013, [http://ec.europa.eu/food/plant/pesticides/guidance\\_documents/docs/app-j\\_en.pdf](http://ec.europa.eu/food/plant/pesticides/guidance_documents/docs/app-j_en.pdf), (last opened 2014-11-02).

### **Contact information:**

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## 6 Annex I: Mathematical Background

### Annex 1

#### The Maximum Dietary Burden Calculation Solved by Linear Programming

In the following section the maximum calculation of residues in fish feed is presented. The program *DietaryBurdenCalculator* considers two fish species with specific requirements (different target nutrition needs) that have to be satisfied.

A possible feed component has three characteristics: a protein content (CP crude protein in % of dry matter (DM)), a lipid content (CL crude lipid in % of dry matter (DM)) and a residue value of a certain substance (for example a STMR value in mg/kg).

This context can be mathematically written as two different linear equations:

$$\begin{aligned}\text{Protein content:} \quad & P_1x_1 + \dots + P_nx_n = P_{\text{Fish}}, \\ \text{Lipid content:} \quad & L_1x_1 + \dots + L_nx_n = L_{\text{Fish}},\end{aligned}$$

where

$P_{\text{Fish}}$ : is the target protein concentration of the diet (%),

$L_{\text{Fish}}$ : is the target lipid concentration of the diet (%),

$P_i$ : is the protein concentration of feed component  $i$  (%),

$L_i$ : is the lipid concentration of feed component  $i$  (%) and

$x_i$ : is the fraction of feed component  $i$  in the diet (-).

For the actual fish diet problem further (trivial) conditions need to be defined in order to solve the mathematical problem:

- $x_i$  must always be between 0 and 1,
- the sum of all  $x_i$  sum always up to 1.

If the idea of a "maximum reasonable balanced" diet (MRBD) is considered, the maximum content of a certain feed may be limited in some cases which can be considered by additional conditions. Therefore the inequalities  $x_i \leq 1$ , for  $i = 1, \dots, n$  are replaced by  $x_i \leq (R_{\text{Fish}})_i$  for  $i = 1, \dots, n$ . The restrictions are constant positive numbers smaller than and may diversify between feed components and fish species by reason of the different nutrition habit.

Obviously, the so far obtained expressions are all linear leading to an infinite number of solutions for the problem with infinite different feed compositions which meet the necessary criteria.

The set of all possible solutions is called feasible solution set.

However, the desired feed composition is that one which results in the maximum concentration for a given feed composition. That corresponds mathematically to the objective function composed by the sum of the products of the part of feed and residue value of the corresponding component.

$$\max S(x) = S_1x_1 + \dots + S_nx_n,$$



where  $S$  is the maximum substance concentration in the diet (mg/kg) and  $S_i$  is the substance concentration of feed component  $i$  (mg/kg). Basically, the method is divided into two steps: Step 1, also called Phase I, is to find a start solution of the problem and Phase II is the improvement of an existing feasible solution until the optimal solution. Dependent on the number and settings of variables the method may either solve the problem exactly or assert that the problem is insolvable.

## Parameter Setting

The following Table 1 shows the protein and lipid needs of two different important aquaculture species reared for human consumption: Rainbow Trout (*Oncorhynchus mykiss*) and Common Carp (*Cyprinus carpio*). A possible feed component data base of the *DietaryBurdenCalculator*

Table 1: Target composition of test diets (%DM) for carp and rainbow trout

Fish Species	CL(%)	CP(%)
Rainbow Trout	15	42
Carp	10	35

rests upon the Working Document of Pesticide Residues in Fish. The data base contains numerous feed components and their lipid content (CL crude lipid in % of dry matter (DM)), their protein content (CP crude protein in % of dry matter (DM)) and partially suggests a Maximum Reasonable Balanced Diet (MRDB) for fish. In the further document we focus on a exemplary data set of five feed components (Table 2).

A classification of feed components can be represented by CC (carbohydrate concentrate), PC

Table 2: Data of several feed components

Category	Feed	CL(%)	CP(%)	Max. % of diet
By-Products	Peanut (meal decorticated)	1	46.5	35
By-Products	Soybean (meal decorticated)	0.8	49.8	40
By-Products	Corn field (Grain meal)	4.8	10.2	35
Cereal Grains/ Crop Seeds	Rice (Broken grains)	0.6	8.1	50
Fat	Vegetable oil (oil)	100	0	10

(protein concentrate) and F (fat). The *DietaryBurdenCalculator* offers the possibility to add three special feed components: fish meal (PC), starch (CC) and oil(F). Table 3 illustrates their protein and lipid content. Additionally these feed components are treated as unloaded feed components and 100% in diet are allowed.

Table 3: Proximate composition of uncontaminated feed components

Feed Component	CL(%)	CP(%)
Fish Meal(PC)	5	75
Starch(CC)	0.1	0.1
Oil(F)	100	0

## Model Functionality

With the program *DietaryBurdenCalculator*, a maximum burden value, the corresponding worst case feed composition and the dietary load of the substance caused by the individual components can be calculated. Further the calculator offers the possibility to modify the residue estimation by adding fish meal (protein concentrate), starch (carbohydrate concentrate), and/or oil (fat) as feed component or by allowing the idea of reasonable diet (MRDB). In general the program offers a high flexibility because the data base of feed components can be changed, two different fish species can be selected and specific residue values can be included. If the dietary burden calculation is not possible, the program informs the user and gives suggestions to solve the problem.

But not only in input but also in output the program offers many possibilities: As a result, the program creates a report that summarizes the input data and results.

## 7 Annex II: Installation of DietaryBurdenCalculator

Installation steps:

