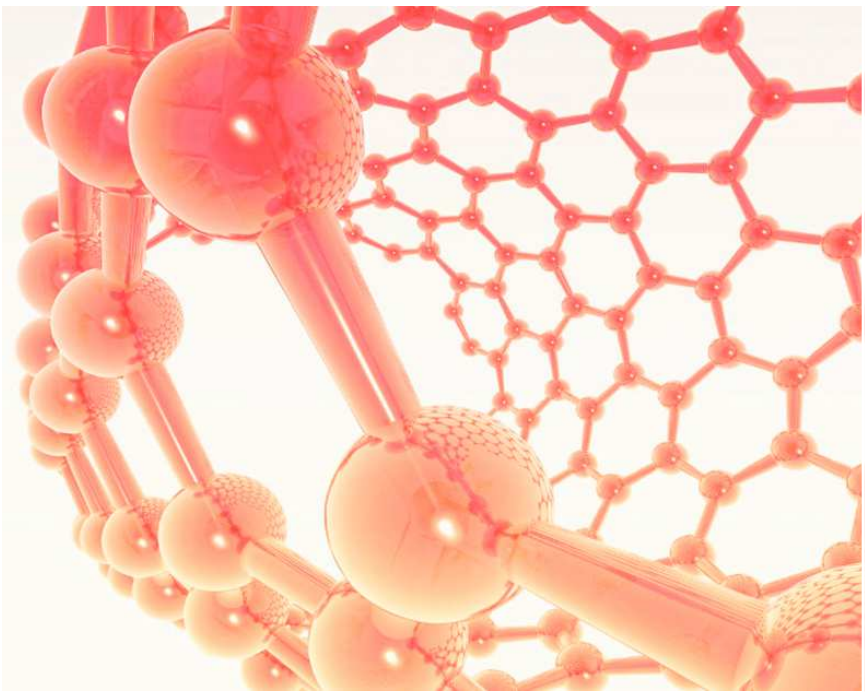
REACHnan

LIFE REACHnano

Development of a web based REACH Toolkit to support the chemical safety assessment of nanomaterials

Guidance on the application of the REACHnano Toolkit



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Guidance on the application of the REACHnano Toolkit

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This technical guidance has been produced by the REACHnano Consortium:

Purpose of the **REACHnano Toolkit** is to offer to companies throughout the supply chain an efficient, innovative and user-friends tool that will help them to comply with REACH Regulation when manufacturing and handling nanomaterials.

The aim of the present **Technical Guideline "Guidance on the application of the REACHnano Toolkit"** developed in the scope of the LIFE REACnano project is to support users on the implementation of the Tool.

With that objective, present Guideline is divided in different parts. Firstly, a brief background explanation introduce the REACHnano project and developed REACHnano Helpdesk in which is implemented the REACHnano Toolkit. Secondly, the objective of the REACHnano Toolkit is presented, followed by the detailed explanation of the REACHnano Toolkit functionalities. Finally, different **CASE STUDIES** are presented as practical operation of the REACHnano Toolkit´s functionalities supporting users on the REACH Regulation implementation.

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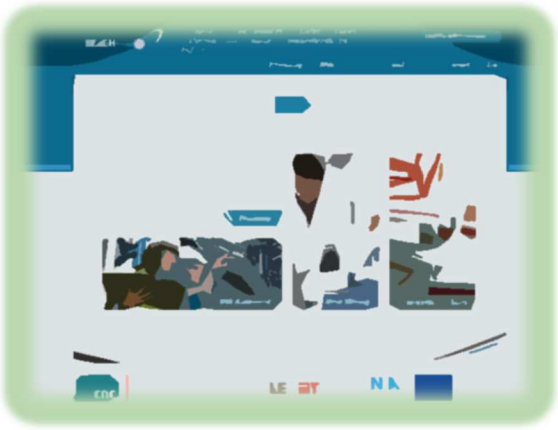


1. Background

Within the context of REACH Regulation, the main issue pertaining to the use of chemicals in whatever size, shape or physical state is to ensure their safety to the human health and the environment. Therefore, since its entry into force on 1 June 2007, REACH plays a central role to ensure the protection of environment and health from risk posed by chemicals and to promote sustainable development. In this context, all available information on the substance has to be gathered and considered for the registration. However, in certain cases, a lack of reliable information exists or even standardized methods, which make difficult the direct application of REACH regulation. This is the case of nanomaterials, which properties are often exceedingly different to those demonstrated by the bulk forms.

In order to address these concerns and considering the priority areas of LIFE +, the main objective of the REACHnano project is to provide innovative instruments to improve the implementation of REACH when manufacturing or handling materials or substances at the nanometer scale, through the development of a web based Help Desk tool to support the risk assessment and promote the safety use of nanomaterials along their life cycle, providing the industry and stakeholders with easy to use tools to support the implementation of REACH regulation.

The **REACHnano Toolkit** developed within REACHnano project, accessible via the REACHnano Helpdesk, takes into account the needs and specifications of end-users and stakeholders, including advanced functionalities that will support industry and authorities to fulfil their main task under REACH. Moreover, this interactive web application will provide an innovative tool to share and exchange information between the scientific community and politicians, enhancing science-policy integration in support of REACH legislation.

2. Objective of the REACHnano Toolkit

The main objective of the 'REACHnano' project is to provide the industry and stakeholders with innovative and easy-to-use tools to support the risk assessment of nanomaterials along their lifecycle. Its goal is thus to support the implementation of the REACH Regulation with regard to nanomaterials manufacturing and handling and ultimately improve the protection of the environment and human health from risk.

The project seeks to consolidate the knowledge base on nanomaterials properties, hazard and exposure and their risk assessment. For that it collects and evaluate the adequacy of the available information on the physicochemical, toxicological and ecotoxicological properties of nanomaterials and related exposure, use and risk management measures.

'REACHnano' develops a complete description of the current exposure scenarios across the nanomaterials lifecycle, covering the existing operating conditions, efficient risk management measures and estimated exposure levels.

With that aims, the final result of the project is a web based Toolkit to support the risk assessment and promote the safety use of nanomaterials along their life cycle. The complete set of innovative tools supporting the risk assessment process, information exchange and the information search process are freely available in the form of a web-based toolkit, being well disseminated widely to stakeholders, including SMEs and competent authorities. This interactive web application also provides an innovative tool to share and exchange information between the scientific community and politicians, enhancing science-policy integration in support of REACH legislation.

3. REACHnano Tool Kit

From the REACHnano Help Desk users can access to the REACHnano Tool kit, as showed in Figure 1. The freely accesibe REACHnano Tool kit´s main functionalities are explained below.

Figure 1. REACHnano Help Desk and linked REACHnano Tool kit Front End.

3.1. Login

Each user may register for free to start using the tool, from the “Sign in” option, as shown in Figure 2.

Figure 2. How to create a user account in the REACHnano Tool kit.

3.2. Main functionalities

Main links of the Reachnano Tool kit are the inventory, risk assessment and social Tool, showed in Figure 3.

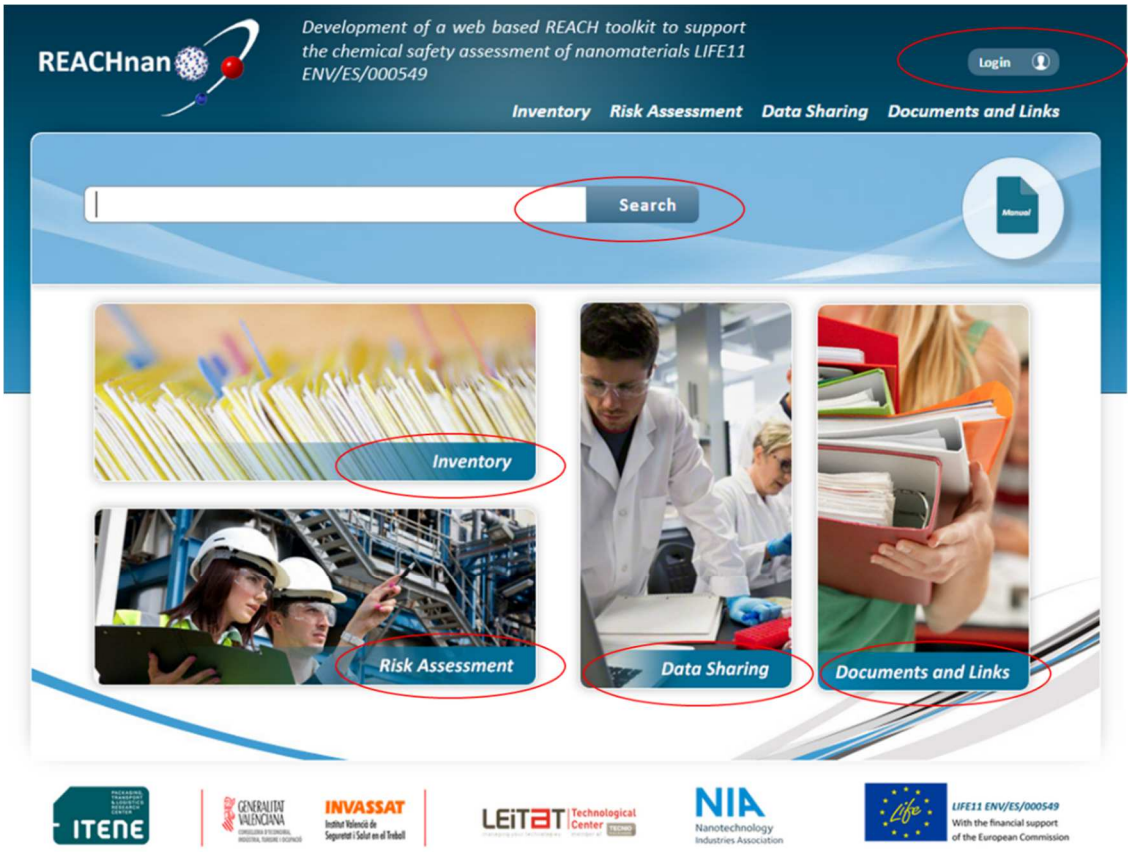


Figure 3. Main functionalities of the Reachnano Tool.

3.2.1. "Inventory"

Access to the database with all the recompiled information on nanomateriales properties, uses, etc. (see Figure 4).

The database has been developed to allow users access to consult and exchange relevant information of most employed nanomaterials (to date, there are information for 30 NMs in the inventory). It is based on a metamodel whose main categories are:

- ✓ General information
- ✓ Classification and Labelling and PBT (persistent, bioaccumulative and toxic) assessment
- ✓ Manufacture, use and exposure
- ✓ Physical and chemical properties
- ✓ Environmental fate and pathways
- ✓ Ecotoxicological information
- ✓ Toxicological information

Each of these categories contains several sets of variables and sub-variables.

Figure 4. Inventory (base of data of nanomaterials).

3.2.2. "Risk Assessment"

This is the access to the environmental and human exposure risk assessment tools.

The environmental risk assessment is done through a model flow analysis probabilistic matter (PMFA). The tool includes all stages of cycle Life of nanomaterials from manufacturing to waste treatment and the model estimates the release of nanomaterials in the air, water and soil as a function of the initial amount.

Because of the paucity of information, the probabilistic models are most useful are the moment. In the probabilistic model, each flow is represented by a probability distribution rather than a fixed value.

In this environmental risk assessment tool, among other parameters, users introduce their tonnage and environmental risk management measures and the tool estimates amount of nanomaterials that is released into each environmental compartment, soil, water and air, as it is shown in Figure X.

Moreover, users can study different exposure scenarios and the tool represent the sum of the total amount released into each compartment (see Figure 5).

Figure 5. Environmental risk assessment tool.

The occupational risk assessment tool (see Figure 6) is based on a combination of control banding approach, exposure estimation tools and new templates of exposure scenarios developed specifically for the case of nanomaterials.

Users may estimate the exposure depending on the operative conditions and applied risk management measures. Once all the necessary data is introduced, the model estimates if one (or more) scenarios can be dangerous for the worker.

Figure 6. Occupational risk assessment tool.

3.2.3. "Data Sharing"

Access to the tool for the introduction of user´s comments and contributions regarding data of inventory, as one of the principals Help desk REACHnano objectives is to promote the exchange of information. In this regard, registered users may share documents with relevant information or data measured on different properties of nanomaterials in the inventory.

Once uploaded the information to the help desk for users, the management team validates the information and then makes available to the public. Information will be available in the database section and in the specific endpoint screen. The nickname of the person and the date will be indicated comment (see Figure 7).

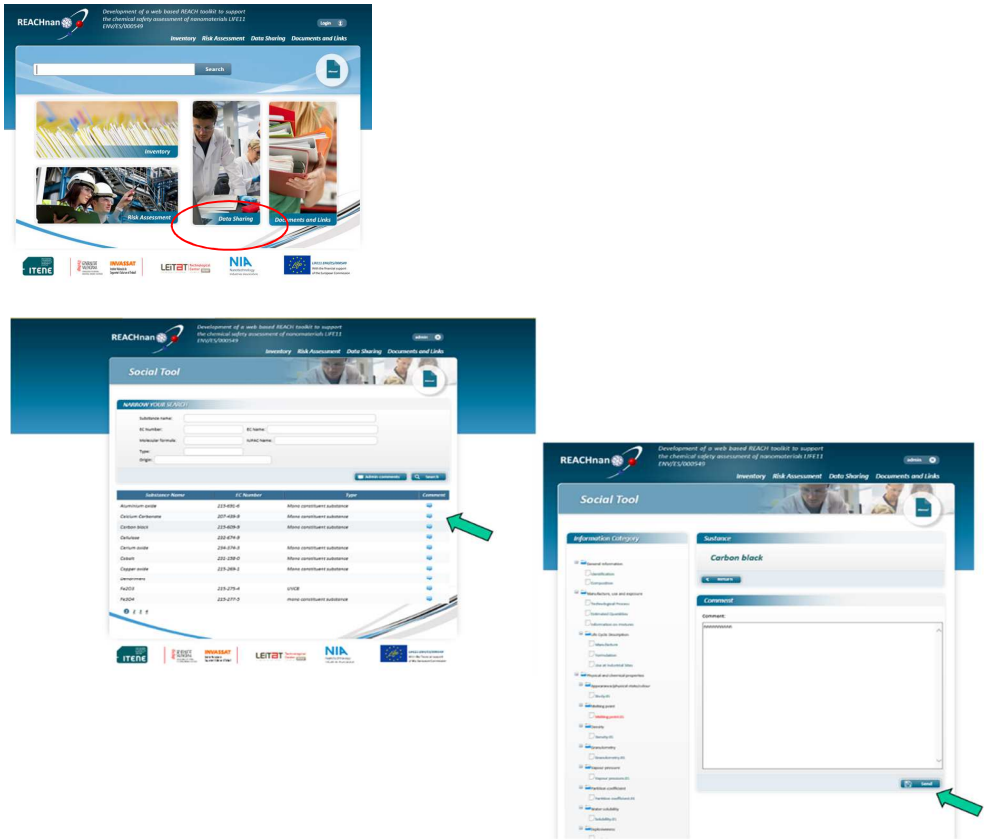


Figure 7. Data Sharing functionalities.

3.2.4. "Documents and links" link

Users can download help documents as manuals, guides, etc. and found links to websites of interest, as shown in figure 8.

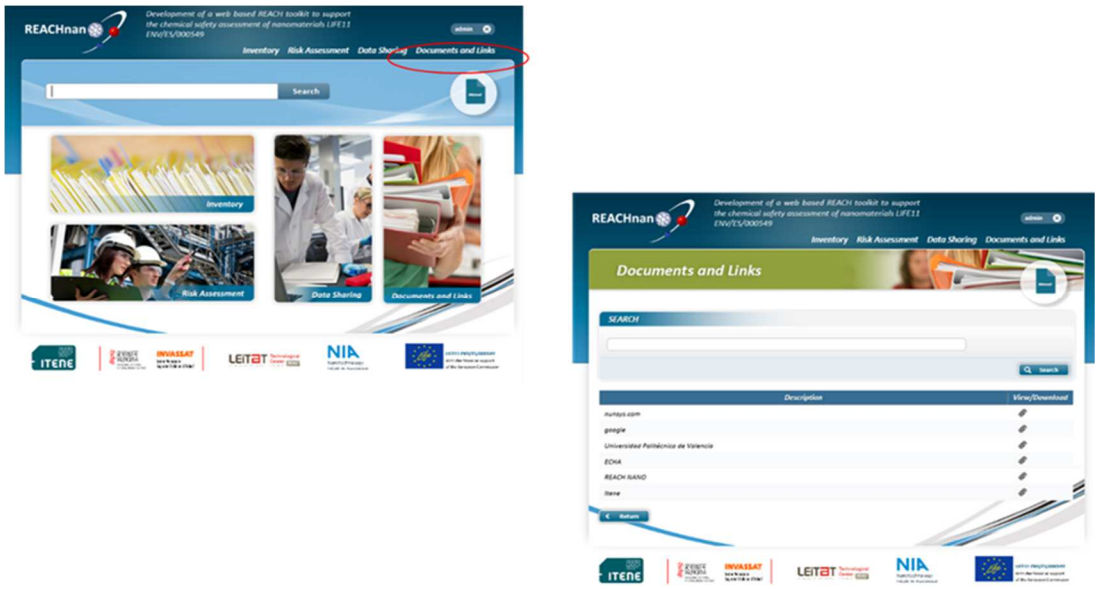


Figure 8. “Documents and links” link.

3.2.5. Search tool

The advanced search tool allows you to find information quickly within the Reachnano Tool kit (see figure 9 and 10).

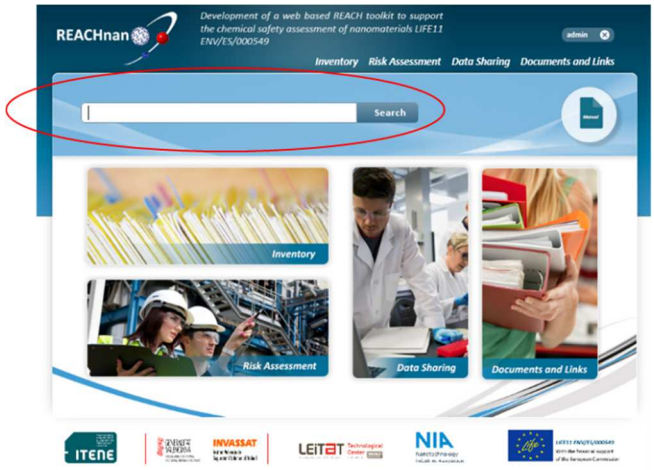


Figure 9. “Search tool” link.

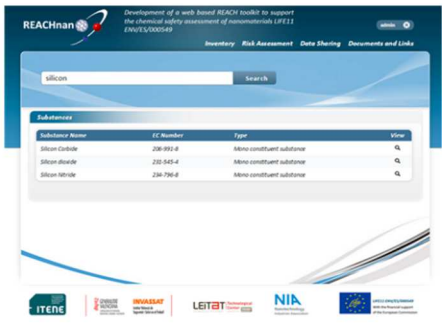


Figure 10. Search list of substances.

4. Practical Case Studies on the use of the REACHnano Toolkit

4.1. Case study on user´s registration and password recovery

Registration to the REACHnano Toolkit is necessary in order to use. The request for access is attended immediately. The tool is freely accessible and information user introduce in it for risk evaluation is totally private. Only information willing to be shared by the user and thus introduced via the Data Share plugging will be published in the inventory after being corroborated and accepted by the tool developers.

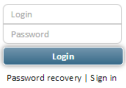
Users registration process is presented in figure 11.

Figure 11. Users registration process.

In the following registration process is explained step by step:

1. From the tool main page, up on the right of the page, access to the login area pressing the command

2. In the login area, you have a specific field to apply for registration. Click over "Sign in" text



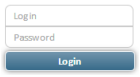
3. A new screen appears, where you have to introduce your user email, nick[1] and password (twice).

4. One data introduced, you have to press "send" button, down on the right of the page

5. In a very short time you will receive an email with the confirmation of successful registry and then you are able to use the tool.

[1] This is the name that will appear when you share information via the Data Share plugging.

6. With your own account created, access again to the login area and introduce your email and password and click button for accessing to the main page of the tool.



7. Once logged, your own “nick” will appear up on the right of the page

8. When willing to log out, only press the cross icon 

9. If you can´t remember your password, you can recover it in any time, only clicking the “password recovery” text in the logging area

4.2. Case study on information searching in the inventory

The REACHnano Toolkit accounts with a searching plugging (see figure 12) permitting you to find any introduced words. The tool searches the word across inventory.

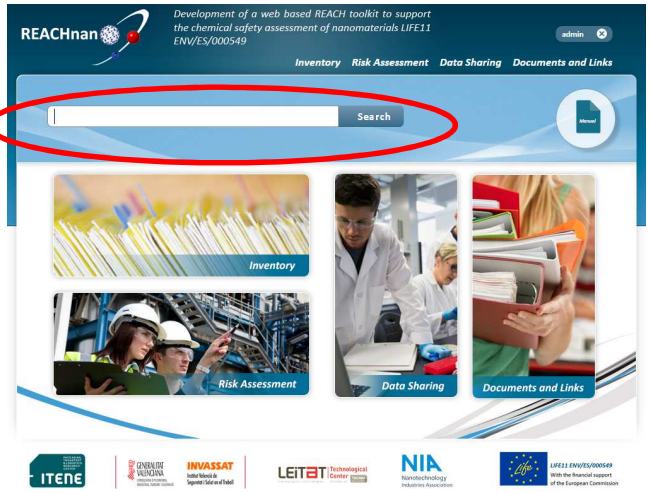


Figure 12. Search plugging.

You only need to introduce the word/words willing to look for and related found out information will appear in the screen.

For example, if you need to find the term “graphene”, introduce the word in the dedicated field and click “search” buttom.

4.3. Case study for inventory use

The access to the inventory is shown in figure 13. In such inventory, reliable information, for of 30 nanomaterials, demanded by REACH regulation when registering chemicals can be found. When you access to this plugging, the list of introduced nanomaterials is presented.

It is possible to search for nanomaterial introducing different parameters: substance name, EC number, EC name, molecular formula, IUPAC name, type or origin and clicking button “Search”.

As example, if you needed information regarding acute oral toxicity of the nanomaterial "silver", you could access to it by introducing in the field "Substance name" the word silver and clicking button "search". Then, you can select the substance from the list clicking on the icon.

Once on the substance information page you can select from the left list the study you are interested in. In this case, acute oral toxicity, you can find three studies (on the left). By clicking on each of them, the detailed information it is shown on the right (see Figure 14).

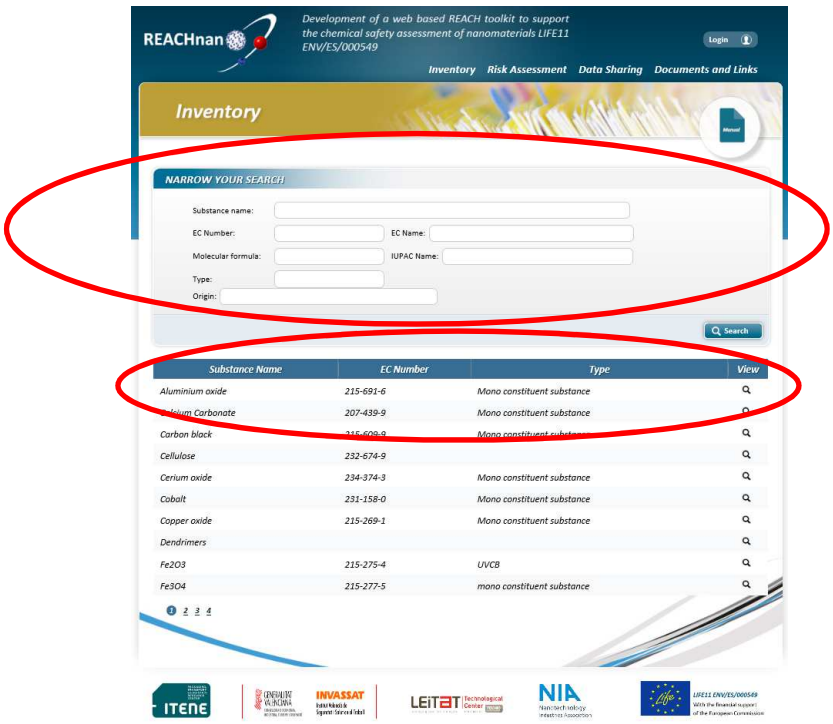


Figure 13. Inventory (base of data of nanomaterials).

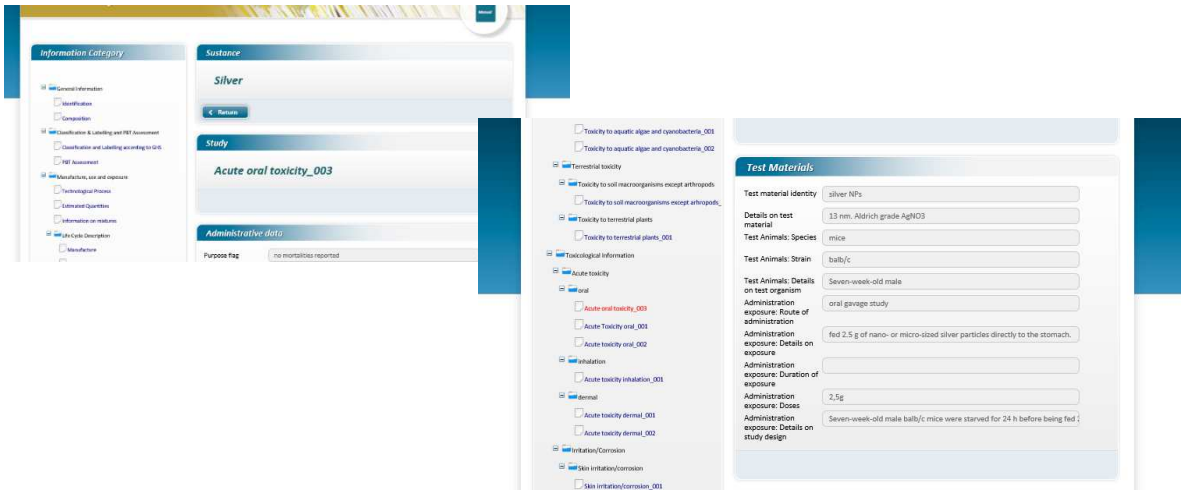


Figure 14. Example of information available of the nanomaterial "silver" from the inventory.

4.4. Case study on Human Risk Assessment

The access for undertake a Human Risk Assessment is summarized in figure 15. When you access by first time to the Tool, no substances will appear in the summary screen as each user generate their own substances of interest and introduce parameters from their own process or activity (see Figure 16).

Figure 15. Occupational risk assessment tool.

Steps to be followed for Risk Assessment are:

1. Create your own substance
2. Access to the substance for Risk Assessment
3. Complete the questionnaire with required information and calculate
4. Check results from your calculations whenever you need in the main screen of listed substances as well as on main screen of Risk assessment tool.
5. Generate the printable template of the estudied exposure scenario.

1. <u>Create your own substance for Risk Assessment</u>

As a first step for Risk Evaluation, you have to create the substance. For that click the "New substance" buttom and a new screen will appear, as shown in Figure 17 with the example of "silver" substance. In that screen you have the option of introduce considered reference values that you can use for Risk Characterization ratio calculation.

Once information is introduced, press "Save button and directly you are taken back to the Summary screen of created substances (see figure 17).

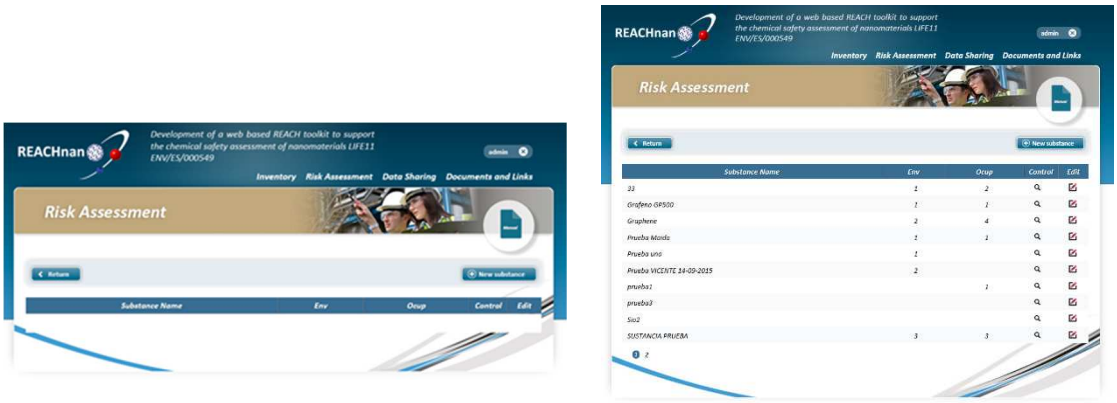


Figure 16. Summary screen for new substance creation (left) and control of the already introduced and studied substances (right).

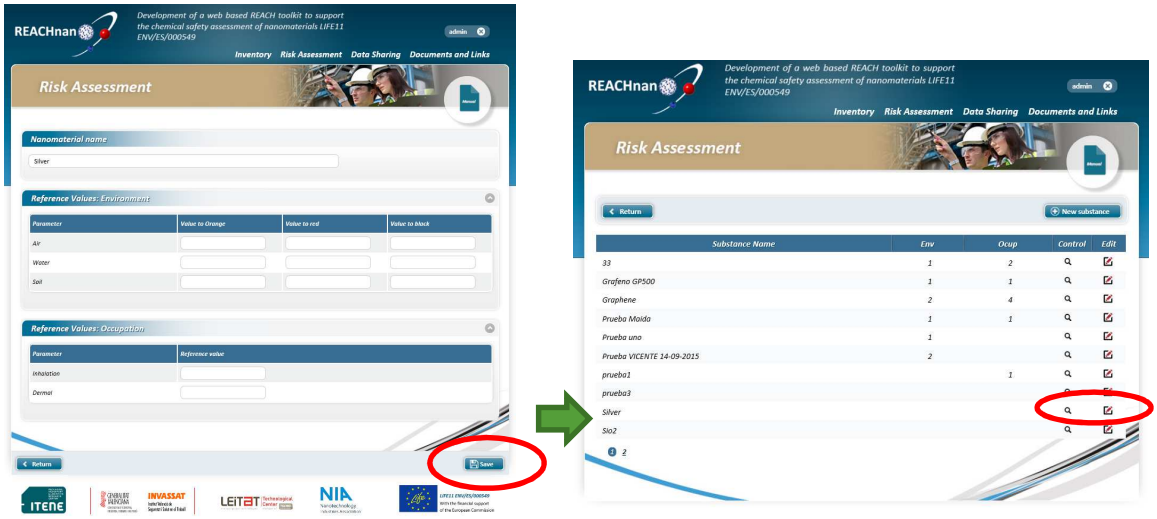


Figure 17. Creation of new substances (left) and selection from the list for Risk Evaluation by pressing "Edit" button (right).

2. Access to the substance for Risk Assessment

Once created the substance, pressing the icon "Edit" you access to the main page of the Risk Assessment, the Control Panel of the substance, with both Human and environmental Risk Assessment tools (see figure 17 on the right).

3. Complete the questionnaire with required information and calculate

In the Control Panel, by pressing the button "New study" on the Human Health Assessment you access directly to a questionnaire asking for different parameters needed for exposure estimation. Once introduced, you have to press "Save and calculate" button and predicted results will be shown (see figure 18).

Figure 18. Creation of new human assessment study (left) and questionnaire to be filled in for human exposure (inhalation and dermal route).

Mandatory fields for the estimation are marked. If no information is introduced on them, the tool notices a message of error. Needed information for exposure estimation is related with operational conditions affecting worker exposure, risk management measures to control worker exposure as well as contextual information on environmental exposure controls (information purpose only).

As an example, if formulating an ink based on graphene, your possible scenario and exposure estimation could be the one shown in figure 19.

If you change the scenario and use a formulation based on 25 % of graphene instead of preliminary 5%, you can observe as exposure estimation is higher, as shown in Figure 20.

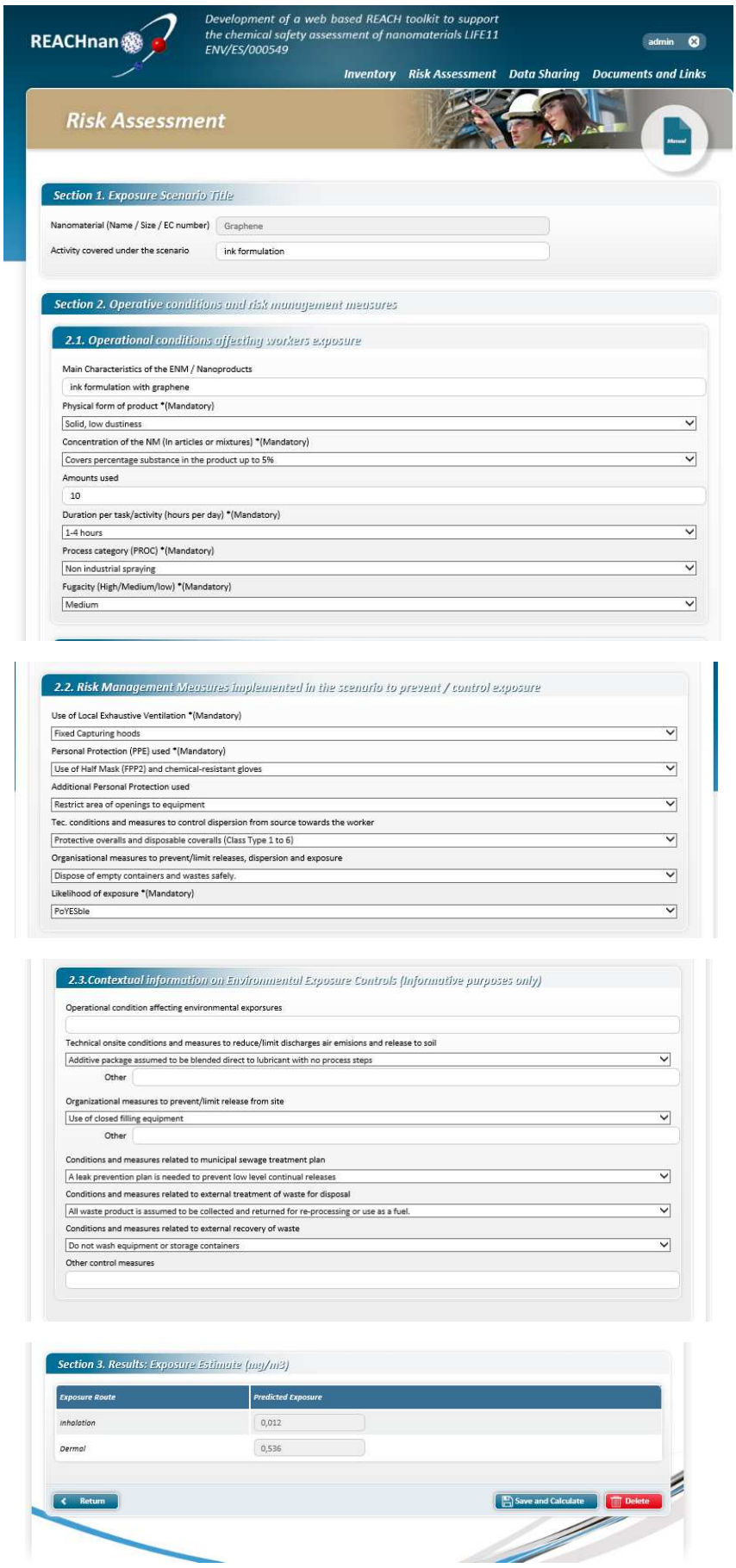


Figure 19. Example of human exposure assessment.

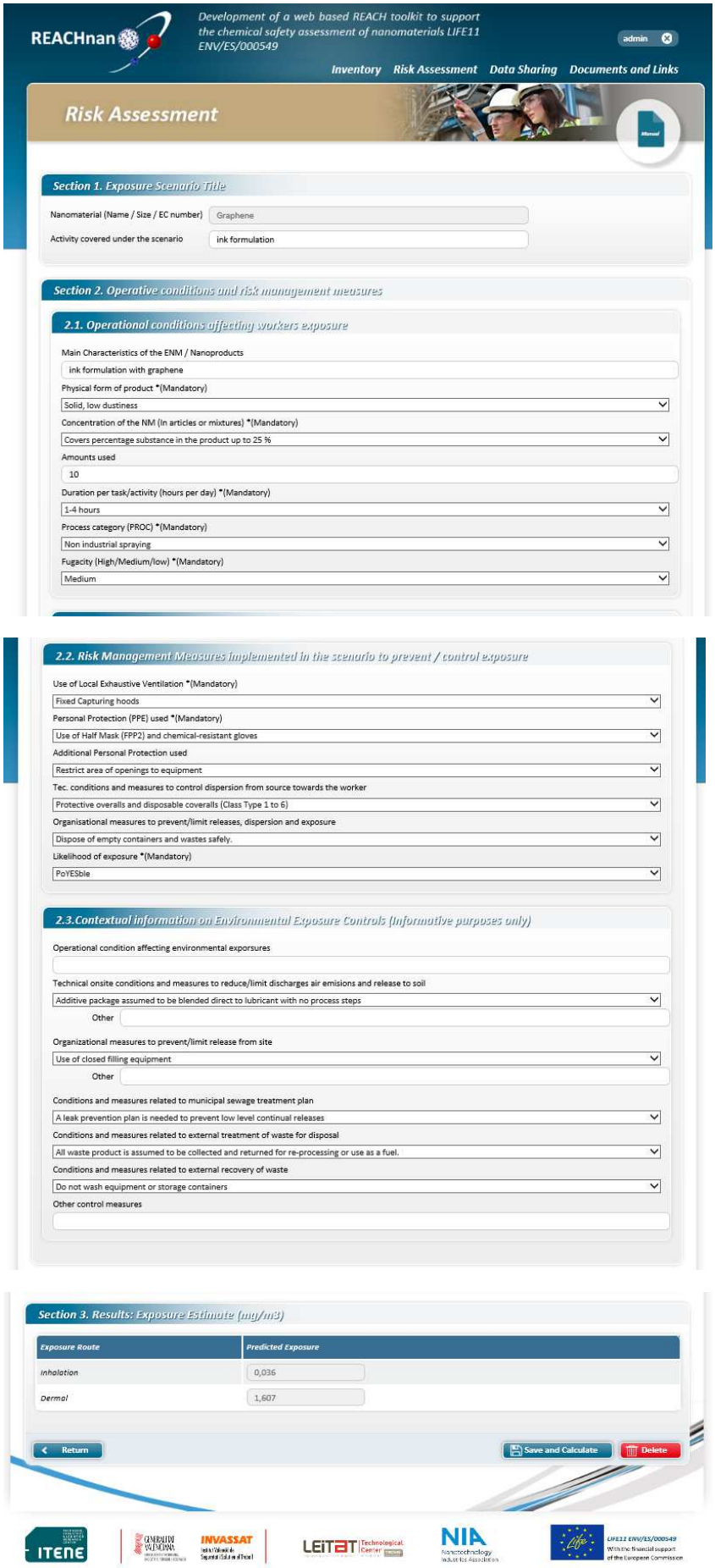


Figure 20. Example of human exposure assessment.

6. Check results

When a result is calculated, by clicking the button “Return” in the page of the questionnaire, you are redirected to a screen where a list as summary of the different undertaken studies is shown (see figure 21, left). If you wish to modify a scenario, you press “Edit” icon and you are redirected to the questionnaire.

Figure 21. Summary screens of studied occupational exposure scenarios: list (left) and control Panel (right).

In this screen you can clearly check different estimation values for each studied exposure scenario (operation). If you click the “Return” button, the Control Panel is shown (see Figure 21, right). The number of studied scenarios is shown on the left (see Figure 22). Moreover, if introduced a reference value for the substance, in that screen it is shown if Risk is under control (green) or not (red color). If not, you are able to return to the scenario and by iteration estimate which are the most suitable risk management measures and operational conditions for exposure reduction until risk is under control.

4.5. Case study on Environmental Risk Assessment

The access for undertake a Human Risk Assessment is summarized in figure 22.

When you access by first time to the Tool, no substances will appear in the summary screen as each user generate their own substances of interest and introduce parameters from their own process or activity (see figure 16), as explained in 4.4.

Steps to be followed for Risk Assessment are, as explined in 4.4. for ocupational exposure:

1. Create your own substance
2. Access to the substance for Risk Assessment
3. Complete the questionnaire with required information and calculate
4. Check results from your calculations whenever you need in the main screen of listed substances as well as on main screen of Risk assessment tool.
5. Generate the printable template of the estudied exposure scenario.

Figure 22. Occupational risk assessment tool.

1. <u>Create your own substance</u>

See 4.4. and figure 22.

2. <u>Access to the substance for Risk Assessment</u>

See 4.4. and figure 22.

3. <u>Complete the questionnaire with required information and calculate</u>

In the Control Panel, by pressing the button “New study” on the Environmental Health Assessment you access directly to a questionnaire asking for different parameters needed for environmental exposure estimation.

Two columns are presented in the questionnaire in order to introduce the data (see figure 23 on the right). Column in the left is for the case of manipulating the nanomaterial itself (i.e. synthesis of the nanomaterial) meanwhile column of the right must be used when a nanobased product is studied (i.e. a cosmetic formulation based on nanoTiO_2).

Once the needed information regarding employed risk management measures and used amount, introduced, by clicking the “Save and calculate” button and predicted results will be shown. the tool estimates the release of the nanomaterial to each of the main environmental compartments /air, water, soil).

As an example, if formulating an ink based on graphene, 10g, using wet scrubber - for dusts, waste gas treatment – absorption, filtration and thermal treatment - Distillation/rectification, your scenario and exposure estimation would be the one shown in figure 24.

If you change the scenario and use 550g instead of preliminary 10g, you can observe as exposure estimation increases, as shown in Figure 25.

Finally, if you use directly 550g of graphene, your exposure varies as shown in Figure 26.

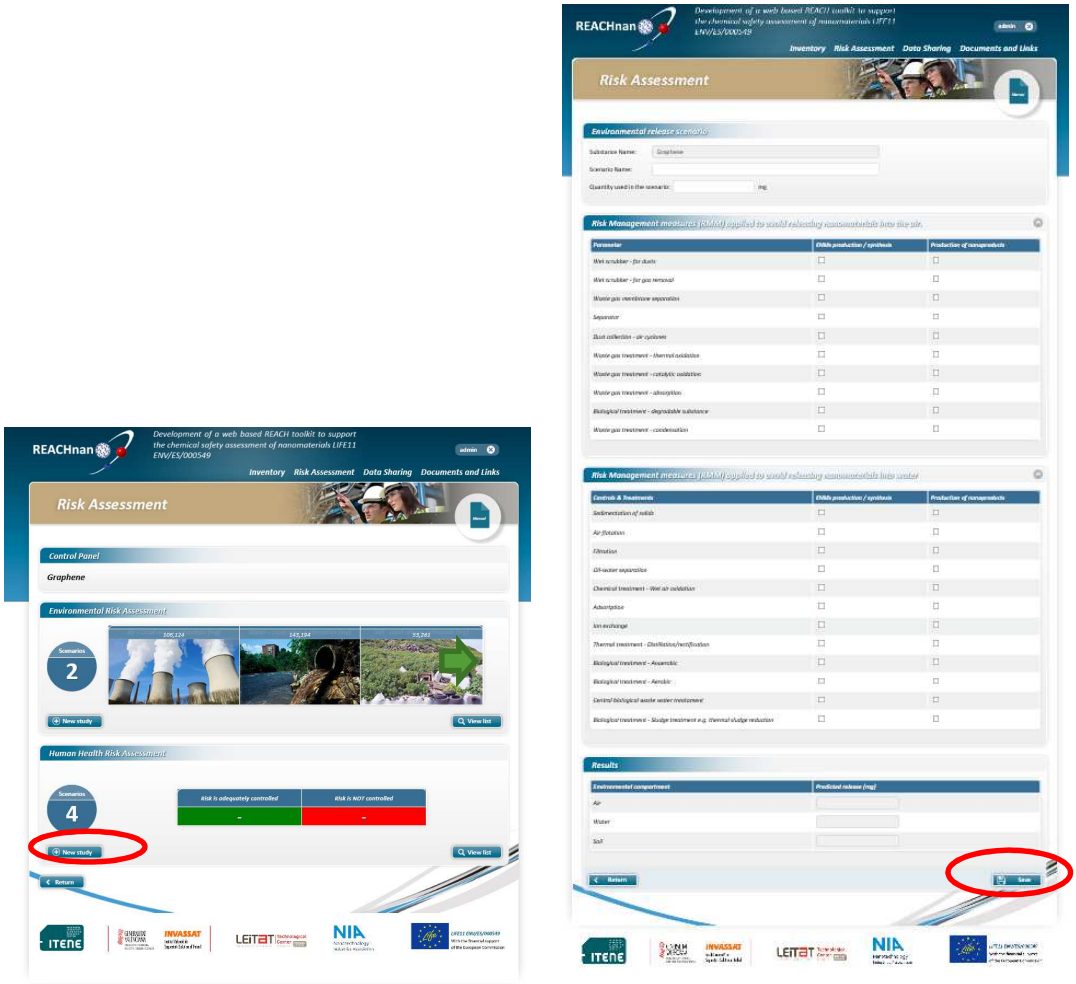


Figure 23. Creation of new environmental assessment study (left) and questionnaire to be filled in for environmental exposure (air, water and soil compartments).

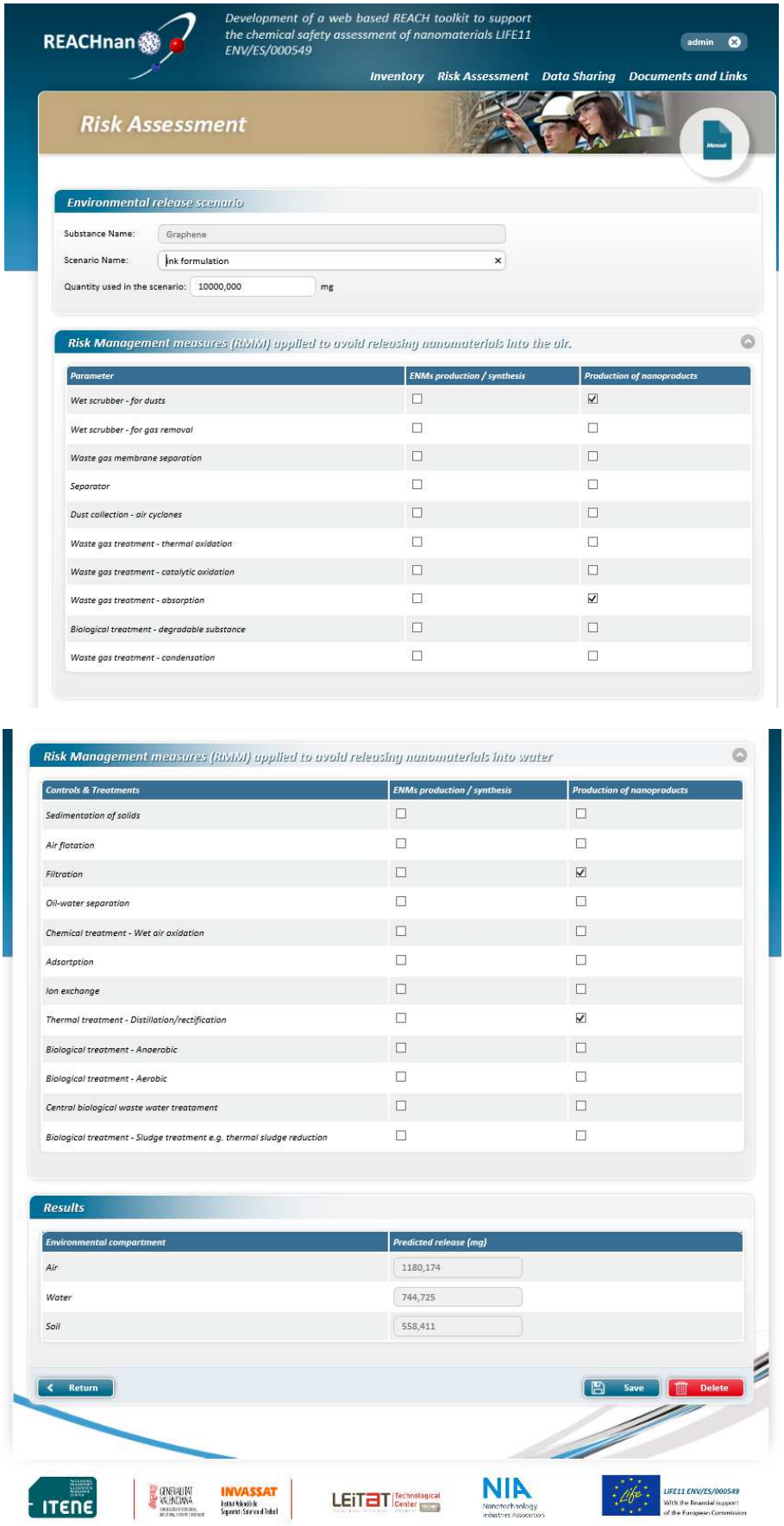


Figure 24. Example of environmental exposure assessment.

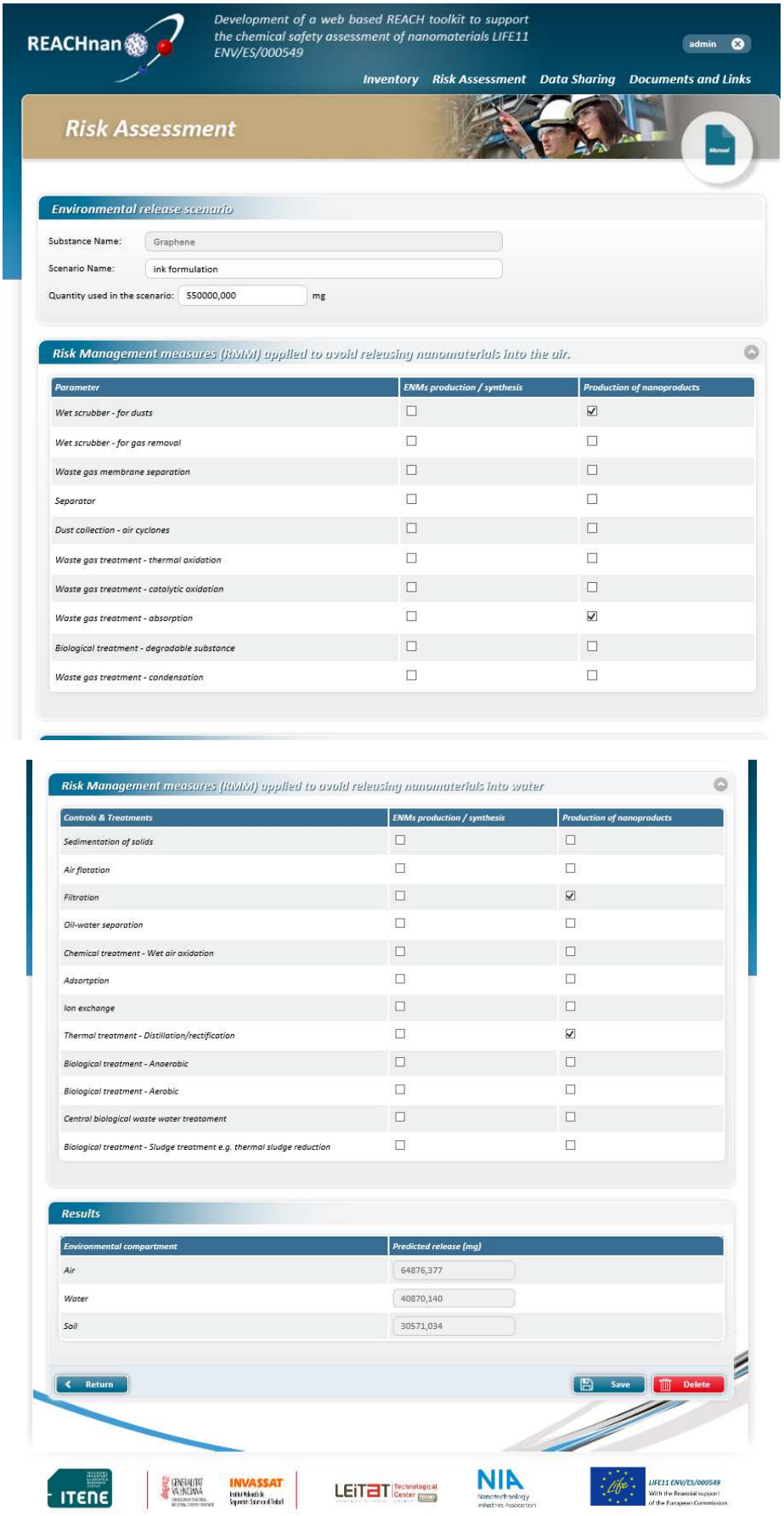


Figure 25. Example of environmental exposure assessment.

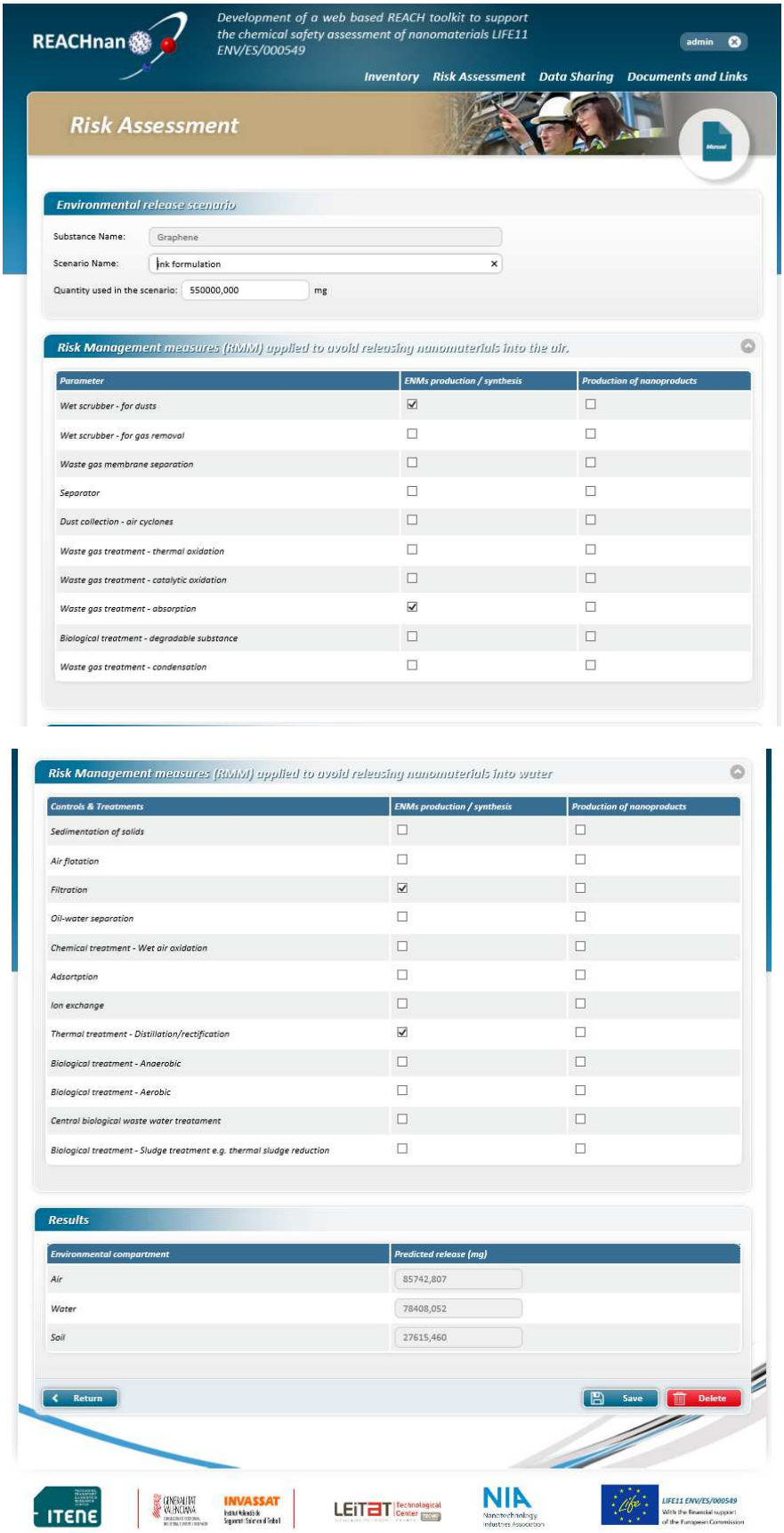


Figure 26. Example of environmental exposure assessment.

4.6. Case study on Data Sharing operation

Access to this module is shown in figure 27.

Figure 27. Data Sharing functionalities.

As a case study, if you are interested in introduce a study of measurement of granulometry of your synthetized nanomaterial ZnO, you have to proceed as explained below:

1. Once logged, access to the "Data Share" plugin. On the "Data share" screen appears a list with the 30 studied nanomaterials.

2. Look for ZnO directly from the list or use the "Narrow your Search" spaces for introduce the key words and press "search" button.

3. Once localized ZnO substance, press icon "Comments" on the right.

4. From information Category list, on the left, select the endpoint "granulometry" and insert your information. Press button "Save".
5. Once the introduced information is checked and approved by the tool development team, your information will appear published in the inventory of ZnO, in the granulometry endpoint, appearing your "nick" and the date the comment was sent.

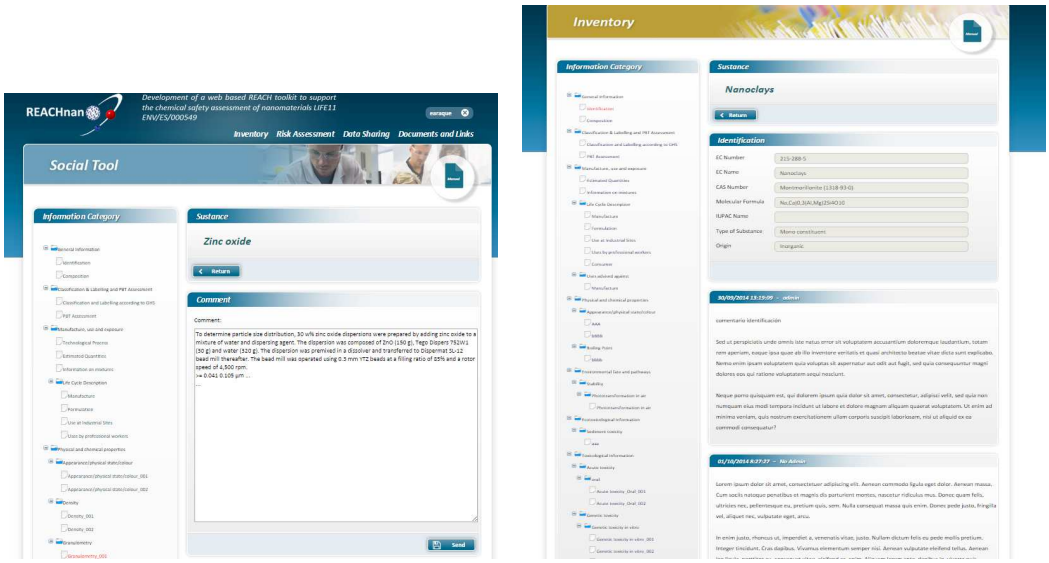


Figure 28. Data sharing case study. On the left, introduction of information (i.e. granulometry of ZnO). On the right, published information (i.e. for nanoclays).

5. References

List of Figures

Further Information

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