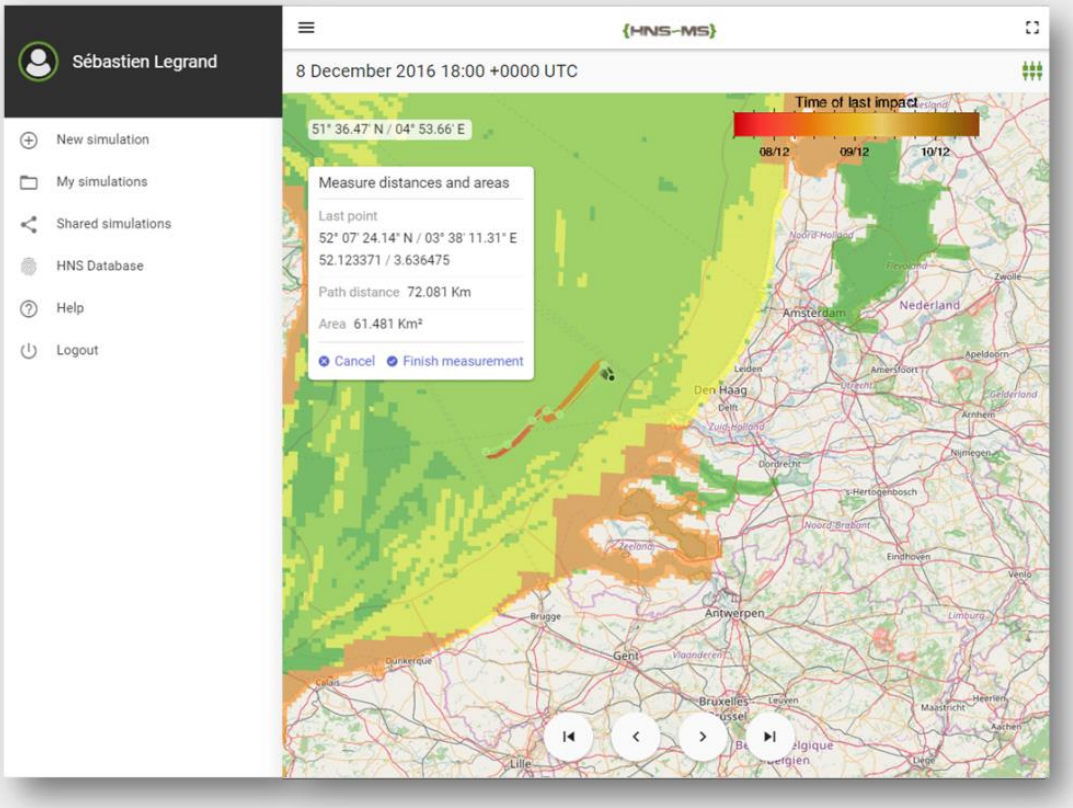
{HNS-MS}

Improving Member States preparedness
to face an HNS pollution of the Marine System

HNS-MS Decision-Support System

User's Guide

HNS-MS final report, part IV



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AND ENVIRONMENT

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About HNS-MS

The European project HNS-MS aimed at developing a decision-support system that national maritime authorities and coastguard stations can activate to forecast the drift, fate and behaviour of acute marine pollution by Harmful Noxious Substances (HNS) accidentally or deliberately released in the marine environment. Focussing on the Greater North Sea and Bay of Biscay, this 27 months project (01/01/2015-31/03/2017) had four specific objectives:

i. To develop a freely accessible data base documenting the most important HNS transported from or to the ports of Antwerp, Rotterdam, Hamburg, Nantes and Bordeaux;
ii. To conduct lab experiments in order to improve the understanding of the physico-chemical behaviour of HNS spilt at sea;
iii. To develop a 3D mathematical modelling system that can forecast the drift, fate and (SEBC) behaviours of HNS spilt at sea. Advanced processes such as chemical reactivity, explosions, fire or interaction with sediment were not considered in this first project;
iv. To produce environmental and socioeconomic vulnerability maps dedicated to HNS that will help end-users assessing the likely impacts of HNS pollution on the marine environment, human health, marine life, coastal or offshore amenities and other legitimate uses of the sea.

All these contributions have been integrated into a web application that will help coastguard stations to evaluate the risks for maritime safety, civil protection and marine environment in case of an acute pollution at sea. HNS-MS has been co-funded by the Directorate-General of European Commission for European Civil Protection and Humanitarian Aid Operations (ECHO).

About this report

This report presents the usages of web-based HNS-MS Decision-Support System developed in the framework of tasks J of the project "HNS-MS – Improving Member States preparedness to face an HNS pollution of the Marine System".

This report is diveded in two part:

- General public tools
- Registered users tools

At the time of writing this report, the tools described were in constant improvement. Some of what follows below may change as future development occurs.

This report is part of a series of 5 technical sub-reports presenting in detail the outcome achieved by the HNS-MS consortium in the framework of this project:

- HNS-MS Layman's report
- Sub-report I : Understanding HNS behaviour in the marine environment
- Sub-report II : Modelling drift, behaviour and fate of HNS maritime pollution
- Sub-report III : Mapping HNS environmental and socioeconomic vulnerability to HNS maritime pollution
- Sub-report IV : HNS-MS Decision-Support System User's Guide

A copy of these reports can be obtained by downloading from the HNS-MS website https://www.hns-ms.eu/publications/.

Contents

Introduction

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1 Introduction

1.1 General context

"*Maritime services have benefited in recent years by considerable expansion fostered by globalization.*"[1] "*Around 90% of world trade is carried by the international shipping industry. Without shipping the import and export of goods on the scale necessary for the modern world would not be possible. Seaborne trade continues to expand, bringing benefits for consumers* across the world through competitive freight costs. Thanks to the growing efficiency of shipping *as a mode of transport and increased economic liberalisation, the prospects for the industry's further growth continue to be strong.*" [2]

If maritime shipping is undoubtedly a key factor of the worldwide economic growth, the constantly growing fleet of tankers, bulk carriers and ever-increasing size container ships exacerbates the risk of maritime accidents, loss of cargoes and acute maritime pollution. In particular, more than 2,000 **harmful or noxious chemical substances** (**HNS**) are regularly shipped in bulk or package forms and can potentially give rise to significant environmental and/or public health impacts in case of spillage in the marine environment.

In recent years, huge efforts have been made by IMO, EMSA as well as other maritime authorities towards greater consideration of these risks. For instance, given the importance and complexity of the matter, the Bonn Agreement, HELCOM, Lisbon Convention, Barcelona Convention/REMPEC, Copenhagen Convention, DG ECHO and EMSA have jointly identified the urgent need of improving preparedness and response to HNS spills (10th Inter-Secretariat Meeting, Helsinki, 27.02.2014).

Until now, preparedness actions at various levels have primarily aimed at classifying the general environmental or public health hazard of an HNS (e.g. development of IBC and IMDG codes; GESAMP profiles), at developing operational datasheets collating detailed, substance-specific information for responders and covering information needs at the first stage of an incident. (MAR-CIS; MIDSIS-TROCS; CAMEO) or at performing a risk analysis of HNS transported in European marine regions (e.g. EU projects HASREP and BE-AWARE). However, contrary to oil pollution preparedness and response tools, only few decision-support systems currently used by Member States authorities (Coastguard agencies or other) integrate 3D models that are able to simulate the drift, fate and behaviour of HNS spills in the marine environment. When they do, they usually rely on black box commercial software or consider simplified or steady-state environmental conditions.

[1] World Trade Organization - https://www.wto.org/english/tratop_e/serv_e/transport_e/transport_maritime_e.htm
[2] International Chamber of Shipping - http://www.ics-shipping.org/shipping-facts/shipping-and-world-trade

HNS-MS aims at developing a 'one-stop shop' integrated decision-support system that is able to predict the drift, fate and behaviour of HNS spills under realistic environmental conditions and at providing key product information - drawing upon and in complement to existing studies and databases - to improve the understanding and evaluation of a HNS spill situation in the field and the environmental and safety-related issues at stake.

The key challenge in this project is to understand the physico-chemical processes that drive the numerous behaviours and fate of HNS spilt in the marine environment.

1.2 What are HNS precisely?

HNS-MS defines **hazardous and noxious substances** or **HNS** following the OPRC-HNS Protocol 2000:

> *"HNS are any substances other than oil which, if introduced into the marine environment, are likely to create hazards to human health, to harm living resources and marine life, to damage amenities or to interfere with other legitimate uses of the sea".*

This generic definition covers a wide range of chemicals with diverse intrinsic qualities (such as toxicity, flammability, corrosiveness, and reactivity with other substances or auto-reactivity). It includes:

- oil derivatives;
- liquid substances which are noxious or dangerous;
- liquefied gases;
- liquids with flashpoints not exceeding 60°C;
- packaged dangerous, harmful and hazardous materials; and
- solid bulk material with associated chemical hazards.

In the framework of HNS-MS, vegetal oils are also considered as HNS.

1.3 How does HNS behave when spilt in the marine environment?

The behaviour of a substance spilt at sea is the way in which it is altered during the first few hours after coming into contact with water. Predicting this behaviour is one of the most important stages in the development of a response strategy.

Since the early 1990's, the best HNS behaviours predictions were given by the Standard European Behaviour Classification (SEBC) [Bonn Agreement, 1991]. This classification determines the theoretical behaviour of a substance according to its density, vapour pressure and solubility. Five main behaviour classes are considered: **gas**, **evaporator**, **floater**, **dissolver** and

sinker. However, most of the time, a substance does not have one single behaviour but rather several behaviours due to its nature and the environmental conditions (wind, waves, current). This is the reason why the SEBC considers a total of 12 mixed behaviours classes (**Error! Reference source not found.**). For example, ethyl acrylate is classified as FED as it floats, evaporates and dissolves.

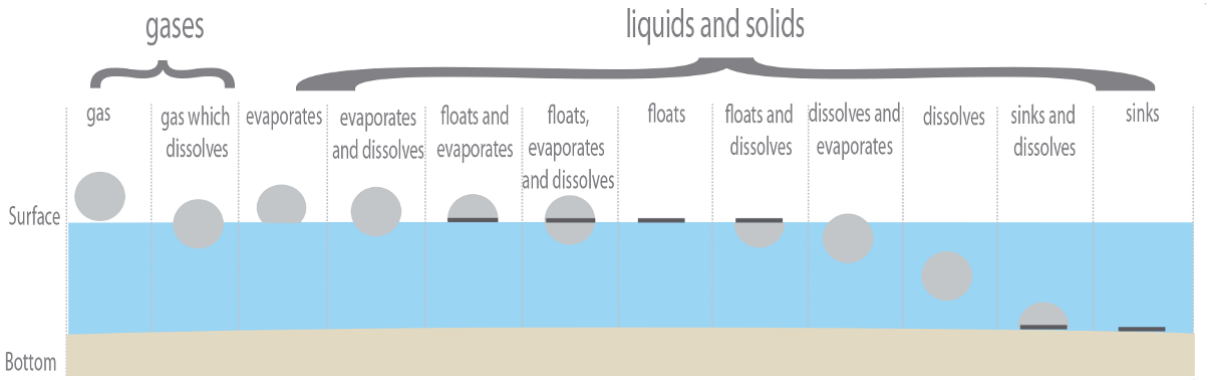

Figure 1: According the Standard European Behaviour Classification (SEBC), a substance spilt at sea will behave following one of these 12 theoretical behaviour classes.

The SEBC code has its limits. It is based on experiments conducted in the laboratory on pure products at a temperature of 20°C in fresh water. These controlled conditions are quite different from those encountered in case of a real incident at sea. In addition, the SEBC also fails to provide any information on the physico-chemical processes explaining the observed mixed behaviour, their kinetics and their eventual competitions. As a consequence, further experimental characterization of chemicals behaviour at different scales (ranging from laboratory to the field) is needed in order to gain a better understanding of the physico-chemical processes at stake, to develop more reliable mathematical models of these processes (taking into account the actual environmental conditions) and eventually to provide more accurate answers to decision makers when they plan response efforts and pollution control.

1.4 HNS-MS objectives

The project HNS-MS aimed at developing a decision-support system that national maritime authorities and coastguard stations can activate to forecast the drift, fate and behaviour of acute marine pollution by Harmful Noxious Substances (HNS) accidentally released in the marine environment.

Focussing on the Greater North Sea and Bay of Biscay, this 2 year project (01/01/2015-31/03/2016) had four specific objectives:

i. To develop a freely accessible data base documenting the most important HNS transported from or to the ports of Antwerp, Rotterdam, Hamburg, Nantes and Bordeaux;
ii. To conduct lab experiments in order to improve the understanding of the physico-chemical behaviour of HNS spilt at sea;
iii. To develop a 3D mathematical modelling system that can forecast the drift, fate and (SEBC) behaviours of HNS spilt at sea. Advanced processes such chemical reactivity, explosions, fire or interaction with sediment were not considered in this first project;
iv. To produce environmental and socioeconomic vulnerability maps dedicated to HNS that will help end-users assessing the likely impacts of HNS pollution on the marine environment, human health, marine life, coastal or offshore amenities and other legitimate uses of the sea.

All these contributions have been integrated into a web application that will help coastguard stations to evaluate the risks for maritime safety, civil protection and marine environment in case of acute pollution at sea.

1.5 HNS-MS workflow

To meet HNS-Ms objectives, the workflow has been subdivided into 10 tasks articulated around 4 main axes (Figure 2):

1. **Lab experiments:** The first axis aims at collating or producing data and information to support the development of the HNS drift and fate model. First a selection of 100+ important HNS transported in the Bonn Agreement area has been performed from a literature and database review. Then, keeping in mind that only processes fully understood can accurately be simulated; several laboratory experiments have be carried out in order to improve our understanding of HNS behaviour both in the water column and at the sea surface. For instance, for the first time, a Lab experiment has been conducted in order to quantify the competition between the evaporation and dissolution kinetics of chemical floating at the sea surface. Finally, two field campaigns have been organised.

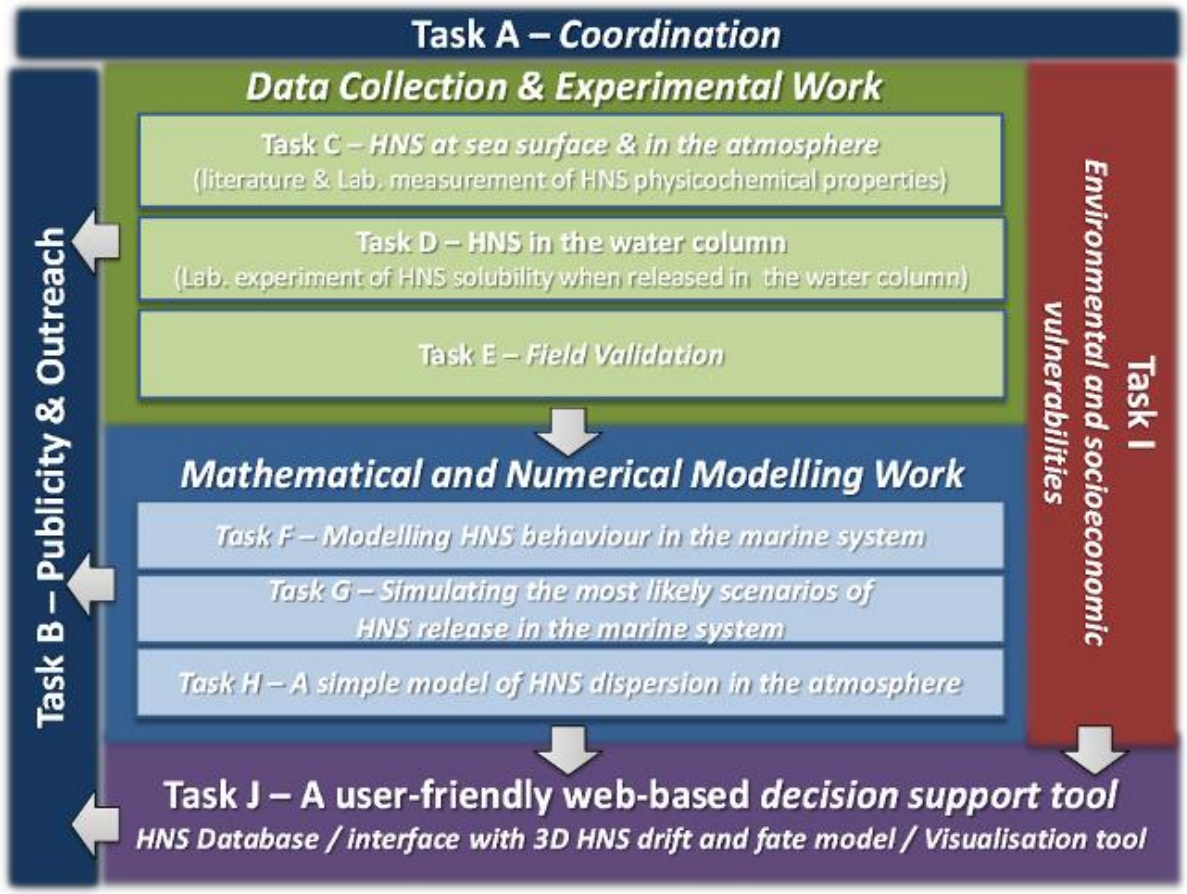

Figure 2: HNS-MS workflow is articulated around 4 main axes: Lab experiments, model development, environmental and socio-economic vulnerabilities mapping and development of a Decision Support System. (Figure from the project proposal submitted to DG-ECHO call to projects 2014)

2. **Mathematical modelling:** The second axis aims at developing a 3D HNS drift and fate modelling software. In order to handle (i) the large variety of HNS physico-chemical properties, (ii) the large variety of possible spillage scenarios and (iii) the large variety of the involved time and space scales, thre different models have been developed, namely
    - ChemSPELL, HNS-MS near-field model
    - ChemDRIFT, HNS-MS far-field model
    - ChemADEL, HNS-MS atmospheric dispersion model
3. **Environmental and socio-economic vulnerabilities:** The third axis aims at developing a series of regional and local vulnerability for HNS-sensitive environmental and socioeconomic features. The HNS-MS vulnerability ranking methodology is mainly an extension of methodology developed in the framework of the BE-AWARE projects, also funded by DG-ECHO.

4. **Decision support System:** Finally, the fourth axis aims at integrating all the previously obtained results in an intuitive, easy-to-use operational web-based HNS decision-support system for the Bonn Agreement area and the Bay of Biscay.

General public tools

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2 General public tools

General public tools are usable by everyone, scientific users or not. They make accessible all static data the project produced.

Three objects are available to the public:

- Vulnerability maps
- HNS-MS database search tool (on the web site)
- JSON REST API

2.1 Vulnerability maps

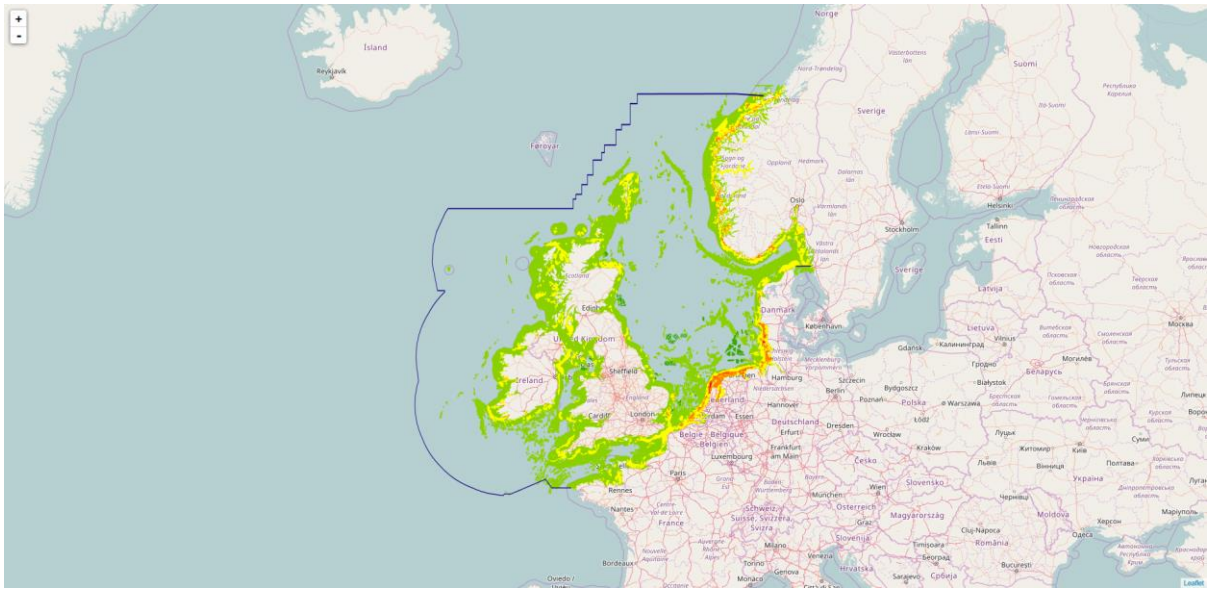


Figure 3 Preview of vulnerability map

Chemicals have a higher negative effect if they are present in a densely populated area (human, animal or vegetal). These effects can also change in intensity depending on the evolution of several parameters.

Aware of that, 74 vulnerability maps were produced. They covers two geographical areas, 5 data types 4 environments and all 4 season.

As the two geographical areas does not share the same selected data types, not all combinations are possible.

Geographical areas:

- Boon Agreement area
- Belgian's north sea area

Data types

- habitats
- protected area
- socio-economic area
- marine projects
- species

Environments

- Air
- Seabed
- Surface
- Water column

2.1.1 Access

Requirement	Internet connection Modern web-browser
Search tool URL	https://www.hns-ms.eu/tools/vulnerability _maps

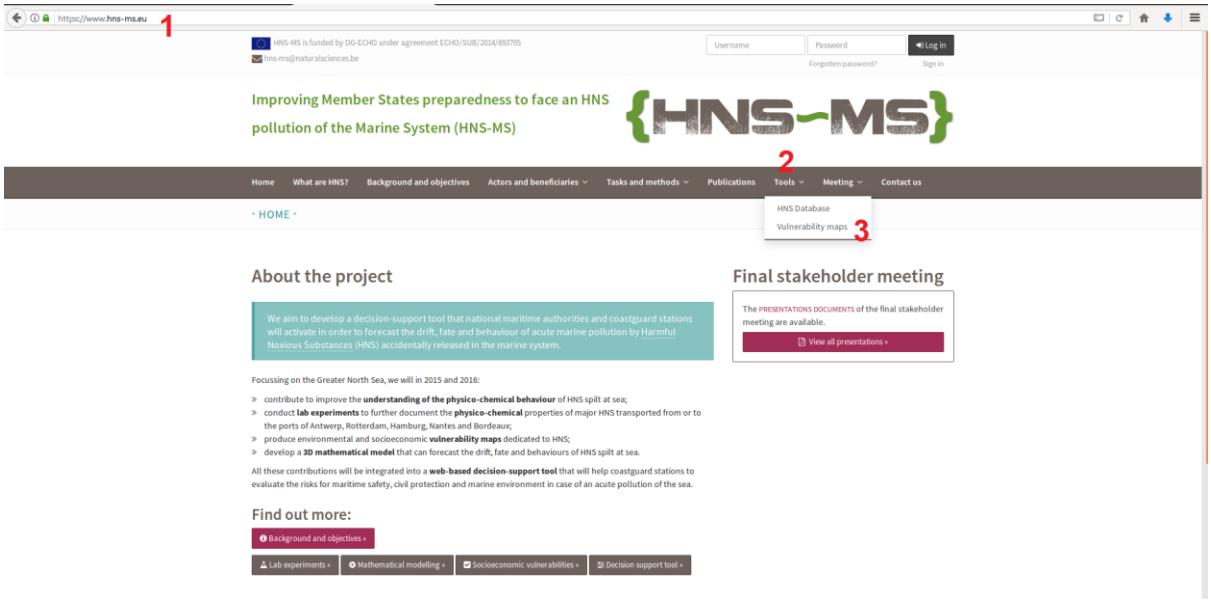


Figure 4 Access to vulnerability maps

Users can access to vulnerability maps via the main menu “Tools”->”Vulnerability Maps”. (Figure 4)

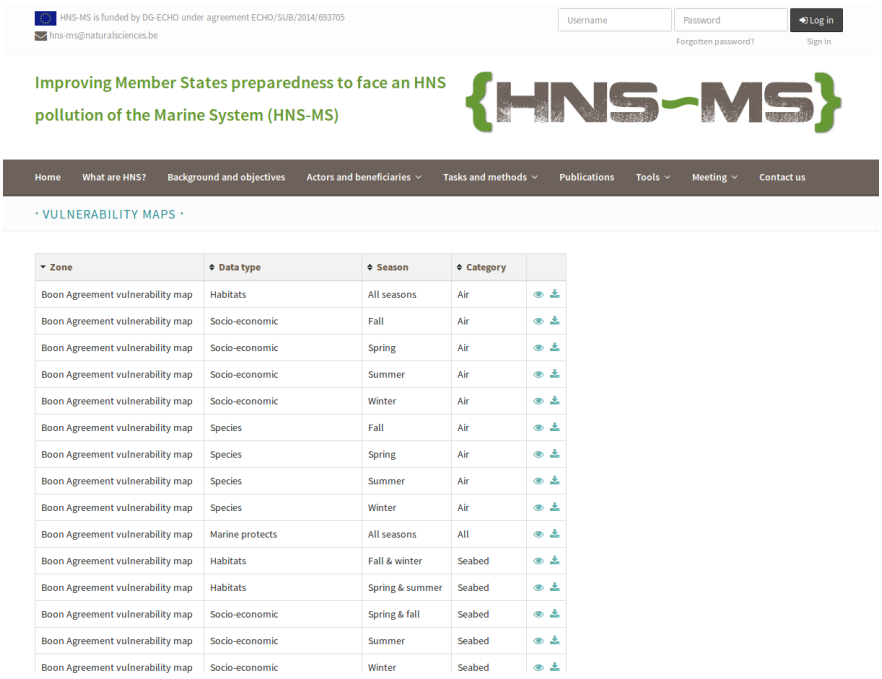


Figure 5 Web page of vulnerability maps

2.1.2 Previsualisation

To facilitate search, the page (Figure 5) give a sortable list of element. By clicking in the header item, sort by alphabetic ( ) or reverse alphabetic ( ) order are possible.

By clicking on the eye button ( ), a previsualisation appears (Figure 3). The user is able to navigate, zoom in and zoom out the map.

2.1.3 Download

Maps can be downloaded one by one in zip file. This file can be imported in any *Geographic Information System* (GIS).

The zip file contain:

- The map in tiling form (Numbered folders)
  It leads to better performance, while maintaining a wide range of zoom.
- An index.html file
  It allows users to have a look at the map without the need of specialized tool. (Internet connection required)
- A metadata.json file
  Allowing import in GIS, correct handle of tiles and giving some useful information like:
  - Map profile (e.g. Mercator)

- Map bounds
- ...

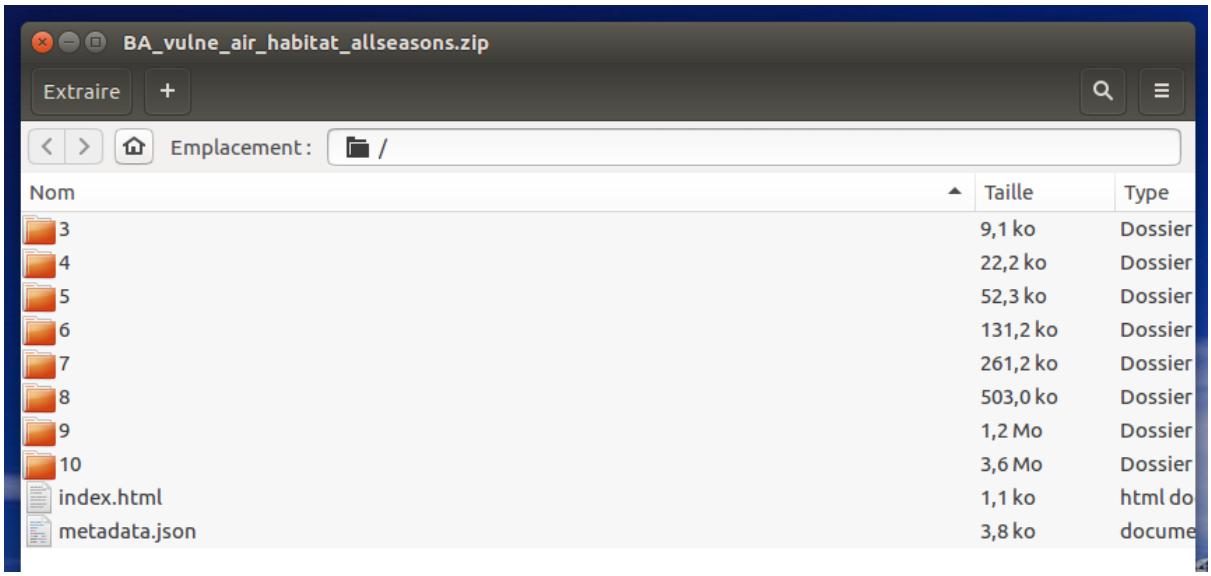


Figure 6 A zip file containing a vulnerability map

2.1.4 List of available maps

Zone	*Data type*	*Season*	*Category*
Boon Agreement vulnerability map	Habitats	All seasons	Air
Boon Agreement vulnerability map	Socio-economic	Fall	Air
Boon Agreement vulnerability map	Socio-economic	Spring	Air
Boon Agreement vulnerability map	Socio-economic	Summer	Air
Boon Agreement vulnerability map	Socio-economic	Winter	Air
Boon Agreement vulnerability map	Species	Fall	Air
Boon Agreement vulnerability map	Species	Spring	Air
Boon Agreement vulnerability map	Species	Summer	Air
Boon Agreement vulnerability map	Species	Winter	Air
Boon Agreement vulnerability map	Marine protects	All seasons	All
Boon Agreement vulnerability map	Habitats	Fall & winter	Seabed
Boon Agreement vulnerability map	Habitats	Spring & summer	Seabed
Boon Agreement vulnerability map	Socio-economic	Spring & fall	Seabed
Boon Agreement vulnerability map	Socio-economic	Summer	Seabed

Boon Agreement vulnerability map	Socio-economic	Winter	Seabed
Boon Agreement vulnerability map	Species	Fall	Seabed
Boon Agreement vulnerability map	Species	Spring	Seabed
Boon Agreement vulnerability map	Species	Summer	Seabed
Boon Agreement vulnerability map	Species	Winter	Seabed
Boon Agreement vulnerability map	Habitats	Fall & winter	Surface
Boon Agreement vulnerability map	Habitats	Spring & summer	Surface
Boon Agreement vulnerability map	Socio-economic	Fall	Surface
Boon Agreement vulnerability map	Socio-economic	Spring	Surface
Boon Agreement vulnerability map	Socio-economic	Summer	Surface
Boon Agreement vulnerability map	Socio-economic	Winter	Surface
Boon Agreement vulnerability map	Species	Fall	Surface
Boon Agreement vulnerability map	Species	Spring	Surface
Boon Agreement vulnerability map	Species	Summer	Surface
Boon Agreement vulnerability map	Species	Winter	Surface
Boon Agreement vulnerability map	Habitats	Fall & winter	Water column
Boon Agreement vulnerability map	Habitats	Spring & summer	Water column
Boon Agreement vulnerability map	Socio-economic	Fall	Water column
Boon Agreement vulnerability map	Socio-economic	Spring	Water column
Boon Agreement vulnerability map	Socio-economic	Summer	Water column
Boon Agreement vulnerability map	Socio-economic	Winter	Water column
Boon Agreement vulnerability map	Species	Fall	Water column
Boon Agreement vulnerability map	Species	Spring	Water column
Boon Agreement vulnerability map	Species	Summer	Water column
Boon Agreement vulnerability map	Species	Winter	Water column
Belgium strategic map	Habitats	All seasons	Air
Belgium strategic map	Habitats	Autumn & winter	Seabed

Belgium strategic map	Habitats	Spring & summer	Seabed
Belgium strategic map	Habitats	Autumn & winter	Surface
Belgium strategic map	Habitats	Spring & summer	Surface
Belgium strategic map	Habitats	Autumn & winter	Water column
Belgium strategic map	Habitats	Spring & summer	Water column
Belgium strategic map	Protected areas	All seasons	All
Belgium strategic map	Socio-economic	Autumn	Air
Belgium strategic map	Socio-economic	Autumn	Seabed
Belgium strategic map	Socio-economic	Autumn	Surface
Belgium strategic map	Socio-economic	Autumn	Water column
Belgium strategic map	Socio-economic	Spring	Air
Belgium strategic map	Socio-economic	Spring	Seabed
Belgium strategic map	Socio-economic	Spring	Surface
Belgium strategic map	Socio-economic	Spring	Water column
Belgium strategic map	Socio-economic	Summer	Air
Belgium strategic map	Socio-economic	Summer	Seabed
Belgium strategic map	Socio-economic	Summer	Surface
Belgium strategic map	Socio-economic	Summer	Water column
Belgium strategic map	Socio-economic	Winter	Air
Belgium strategic map	Socio-economic	Winter	Seabed
Belgium strategic map	Socio-economic	Winter	Surface
Belgium strategic map	Socio-economic	Winter	Water column
Belgium strategic map	Species	Autumn	Seabed
Belgium strategic map	Species	Spring	Seabed
Belgium strategic map	Species	Summer	Seabed
Belgium strategic map	Species	Winter	Seabed
Belgium strategic map	Species	Autumn	Surface
Belgium strategic map	Species	Spring	Surface
Belgium strategic map	Species	Summer	Surface
Belgium strategic map	Species	Winter	Surface
Belgium tactic map	Habitats & Protected areas	All seasons	All
Belgium tactic map	Socio-economic	All seasons	All
Belgium tactic map	Species & Marine protected areas	All seasons	All

2.2 HNS-MS database search tool

Chemicals are all different, some make more damages when at sea than on the beach, some exactly the opposite. The purpose of this search tool is to give important information on HNS in terms of toxicity, physical and chemical parameters.

To facilitate access to normal users, scientists or not, an easy to use search tool is provided on the web site.

This tool allow research by four parameters:

- Name (760+ synonyms)
- SEBC Behaviour (floater, dissolver, …)
- CAS Number
- UN Number

Assuming some chemicals could have complex names; the search tool is able to work with a part of it and guide the users to the right substance. This feature also work with a part of SEBC Behaviour, CAS Number and UN number.

In case of unsuccessful search, the tool invite the users to go to other websites (Figure 7).

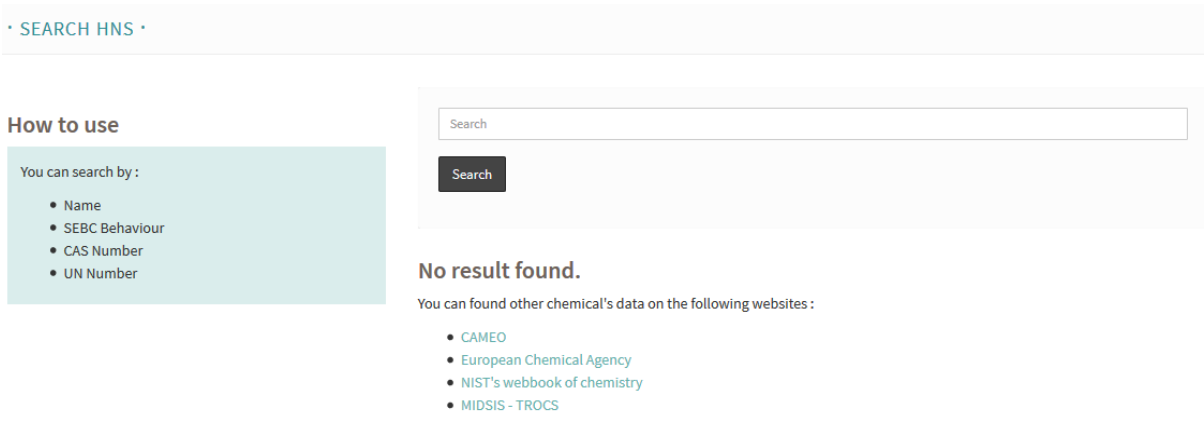


Figure 7 Unsuccessful search

2.2.1 Access

Requirement	Internet connection Modern web-browser
Search tool URL	https://www.hns-ms.eu/hnsdb/

The HNS database search tool is also accessible via the main menu “Tools”->”HNS Database”. (Figure 8)

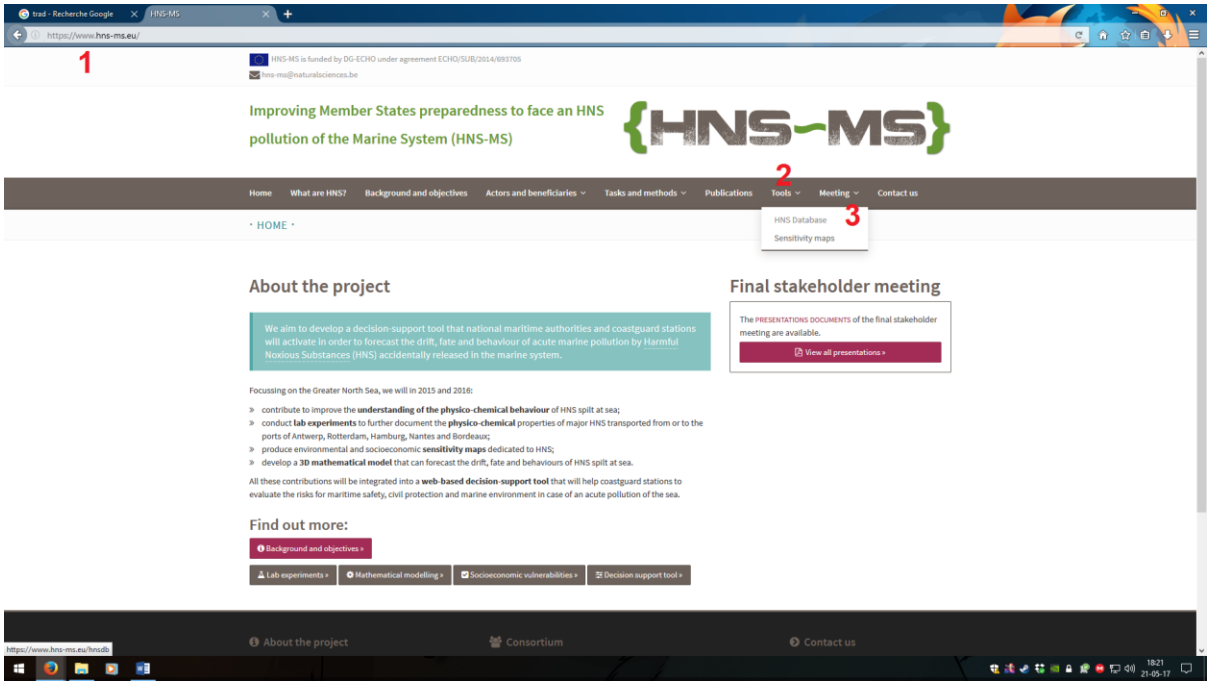


Figure 8 Where to find the search tool ?

Example of usage:

Let us search information about the chemical called "2-Hydroxy-2-Methylpropanenitrile" also called "Acetone Cyanohydrin".

1. Go to the search tool
    a. By direct URL : https://www.hns-ms.eu/hnsdb/
    b. Or via the menu bar (see Figure 8)

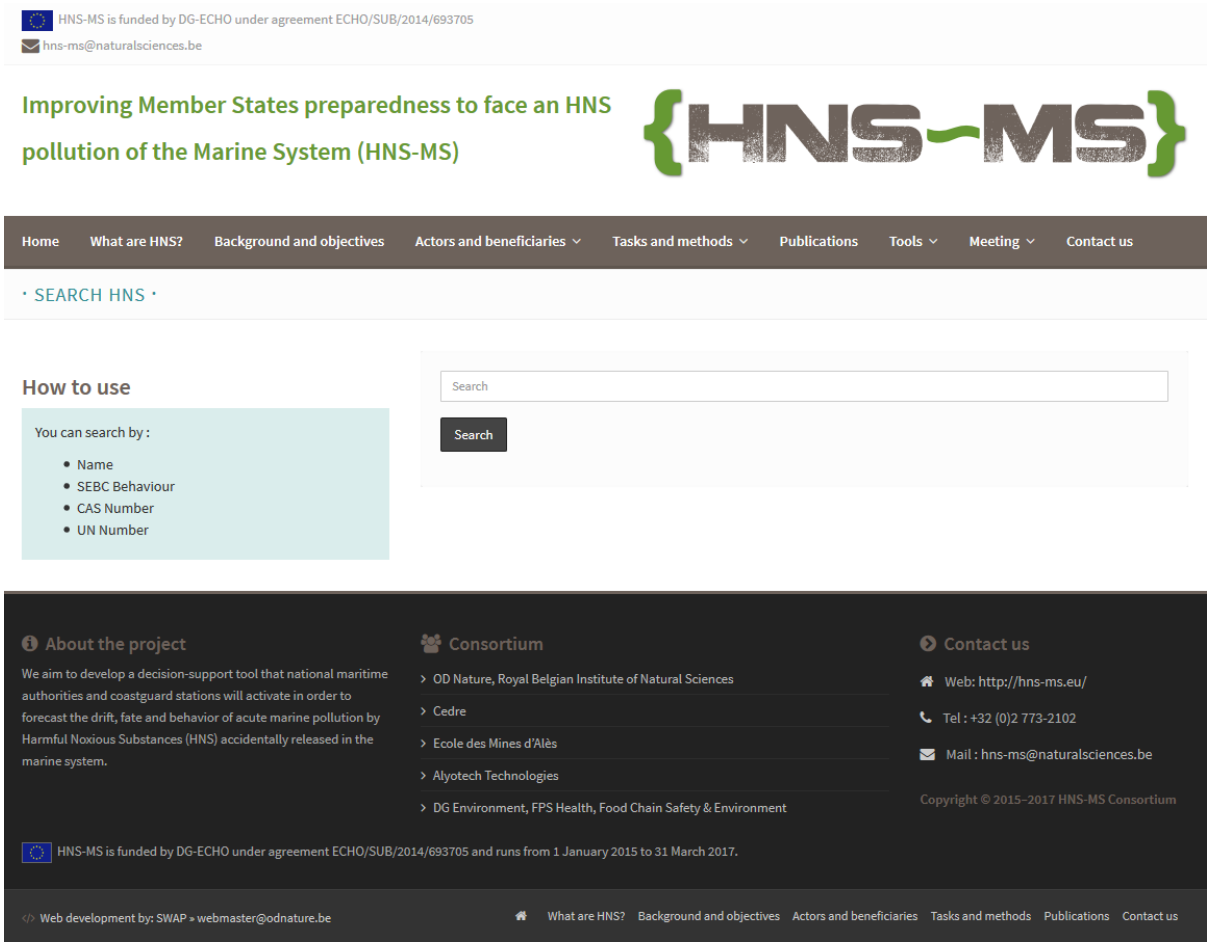
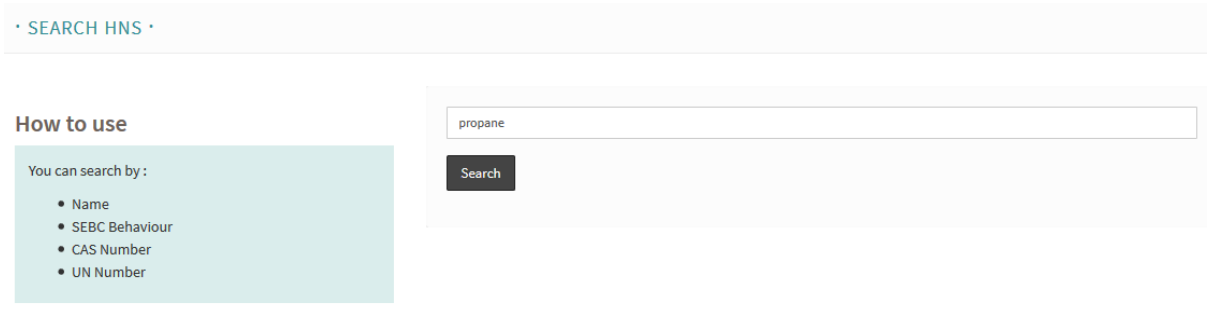
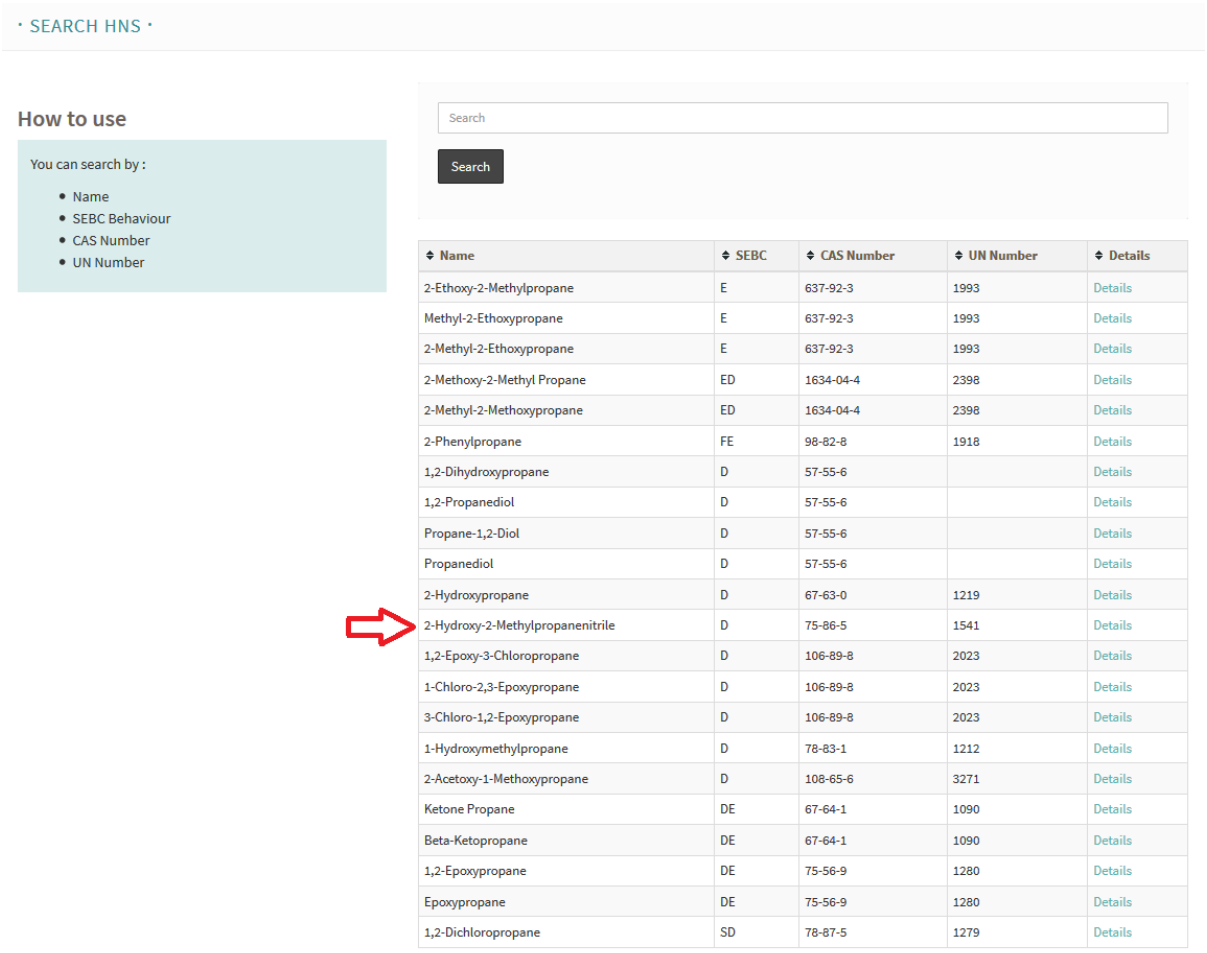


Figure 9 The search tool on the web site

2. In the "Search" field type a part of the name (e.g. "propane")



3. By clicking on the search button, a list of available HNS is displayed.
   By default, the results are not sorted. The user can change the sorting by clicking on the column name he wants to sort.



Name	SEBC	CAS Number	UN Number	Details
2-Ethoxy-2-Methylpropane	E	637-92-3	1993	Details
Methyl-2-Ethoxypropane	E	637-92-3	1993	Details
2-Methyl-2-Ethoxypropane	E	637-92-3	1993	Details
2-Methoxy-2-Methyl Propane	ED	1634-04-4	2398	Details
2-Methyl-2-Methoxypropane	ED	1634-04-4	2398	Details
2-Phenylpropane	FE	98-82-8	1918	Details
1,2-Dihydroxypropane	D	57-55-6		Details
1,2-Propanediol	D	57-55-6		Details
Propane-1,2-Diol	D	57-55-6		Details
Propanediol	D	57-55-6		Details
2-Hydroxypropane	D	67-63-0	1219	Details
2-Hydroxy-2-Methylpropanenitrile	D	75-86-5	1541	Details
1,2-Epoxy-3-Chloropropane	D	106-89-8	2023	Details
1-Chloro-2,3-Epoxypropane	D	106-89-8	2023	Details
3-Chloro-1,2-Epoxypropane	D	106-89-8	2023	Details
1-Hydroxymethylpropane	D	78-83-1	1212	Details
2-Acetoxy-1-Methoxypropane	D	108-65-6	3271	Details
Ketone Propane	DE	67-64-1	1090	Details
Beta-Ketopropane	DE	67-64-1	1090	Details
1,2-Epoxypropane	DE	75-56-9	1280	Details
Epoxypropane	DE	75-56-9	1280	Details
1,2-Dichloropropane	SD	78-87-5	1279	Details

4. We have found our targeted chemical in the list.
   By clicking on the blue label “Details”, the user will access to the detailed information about the HNS.

2.2.2 Detailed information page

The detailed information page is identical on the web site and web app and is divided in 7 sections.

Quick navigation is possible. By clicking on the blue button (under the name of the HNS - Figure 10) with the section name, the associated section will be displayed. Return to the top of the page is done by clicking on the "Top^" button on the right of section title bar.

1. Description (Figure 10)
   Summary of chemical classifications and synonyms.
2. GHS Security Information (Figure 10)
   Labelling of the HNS according to the Globally Harmonised System of Classification and Labelling of Chemicals (GHS)

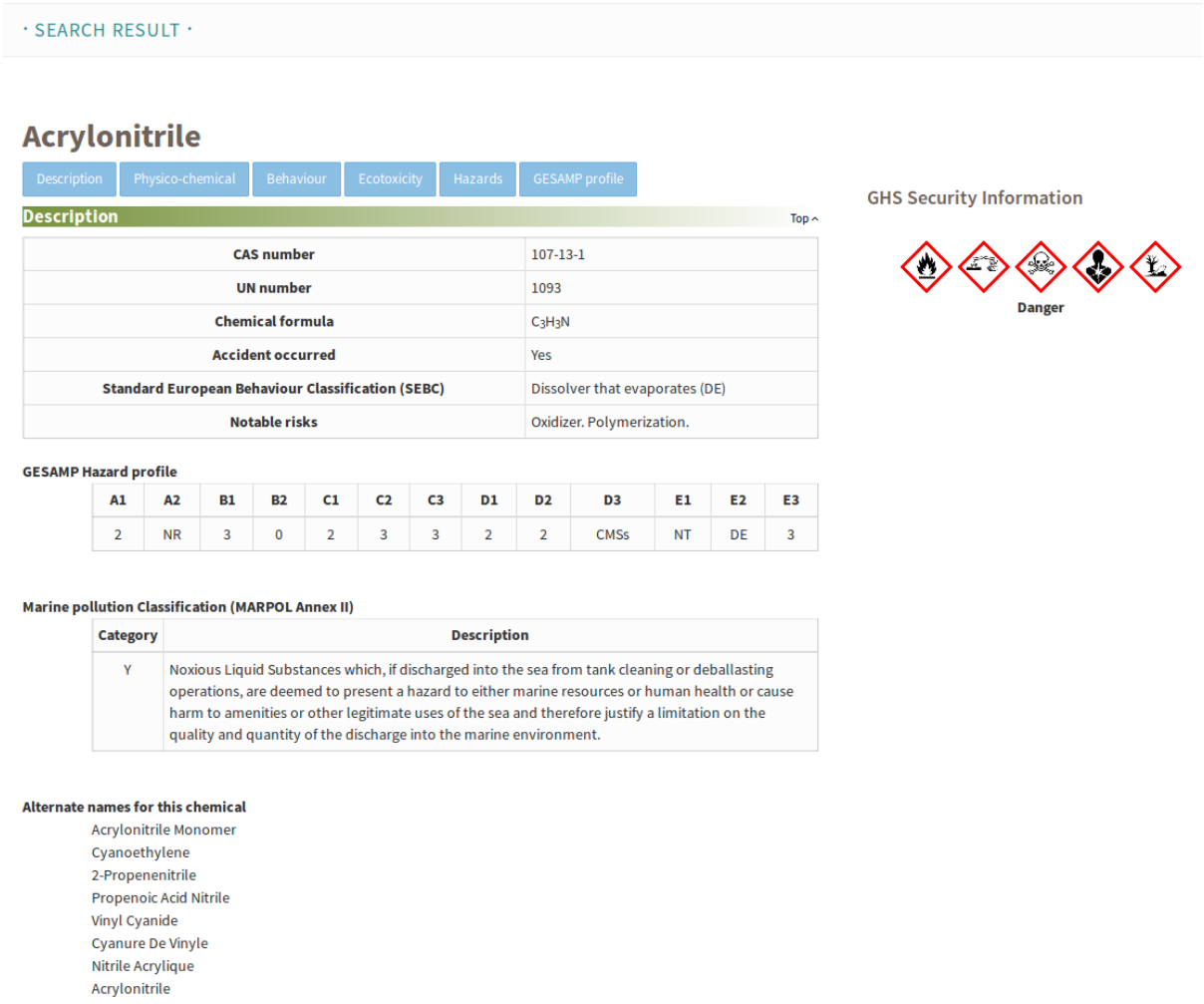


Figure 10 Description and GHS Security Information

3. Physico-chemical properties

List of physical and chemical parameters.

Physico-chemical properties Top

Chemical formula	C_3H_3N
Molar mass	53.06 [g/mol]
Critical molar volume	0.000173 [m^3/mol]
State	Liquid at 25°C and 1 atm
Fusion temperature	-83 [°C]
Boiling temperature	77.4 [°C]
Critical temperature	540 [°C]
Density	810 [Kg/m^3] at a temperature of 20°C
Surface tension	27.22 [mN/m] at a temperature of 20°C
	26.63 [mN/m] at a temperature of 25°C
Kinematic viscosity	0.43 [cSt] at a temperature of 20°C
	0.42 [cSt] at a temperature of 25°C
Hydrosolubility	79000 [mg/l] at a temperature of 20°C and salinity of 0‰
Vapour pressure	11500 [Pa] at a temperature of 20°C
	14470 [Pa] at a temperature of 25°C
Critical pressure	4660000 [Pa]
Vapour density	1.9
Flash point (Pensky-Martens closed cup)	-1 [°C]
Lower explosivity limit (LEL)	3 [%]
Upper explosivity limit (UEL)	17 [%]
Vaporization enthalpy	616000 [J/Kg] at a temperature of 77.4°C
Combustion enthalpy	31900000 [J/Kg]
Specific heat capacity	2050 [J/(Kg·K)]
Combustion efficiency	98 [%]
Mass flow rate of the combustion surface	0.05 [Kg/(m^2·s)]
Radiative fraction	26 [%]
Henry's constant	8.7 [mol/(m^3·Pa)]

Figure 11 Physico-chemical properties

4. Behaviour

   Information about the behaviour in aquatic environment.

Behaviour Top

Log Kow	-0.92
Log Koc	-0.07
Hydrolysis (Half-life)	Not hydrolysable
Aqueous photolysis (Half-life)	Not photolysable
Biodegradation in estuary environment (Half-life)	Not biodegradable
Biodegradation in marine environment (Half-life)	Not biodegradable
Standard European Behaviour Classification (SEBC)	Dissolver that evaporates (DE)
Bioconcentration factor (BCF)	1

Figure 12 Behaviour

5. Ecotoxicity

   Information about toxicity in aquatic environment.

Ecotoxicity Top

Lowest median lethal concentration (LC_{50}) on algae	1.63 [mg/l]
Lowest median lethal concentration (LC_{50}) on crustacean	6 [mg/l]
Lowest median lethal concentration (LC_{50}) on fishes	5.16 [mg/l]
Highest no observed effect concentration (NOEC) on algae	0.8 [mg/l]
Highest no observed effect concentration (NOEC) on crustacean	0.5 [mg/l]
Highest no observed effect concentration (NOEC) on fishes	0.17 [mg/l]
Assessment factor (AF)	100 on the short-term
	100 on the long-term
Predicted No Effect Concentration (PNEC)	16.3 [µg/l] on the short-term
	1.7 [µg/l] on the long-term

Figure 13 Ecotoxicity

6. Hazards

Labelling, hazards (H) and prevention (P) statement according to the Globally Harmonised System of Classification and Labelling of Chemicals (GHS)

Hazards

Top

Danger

IDLH	85 [ppm]

Hazards statements

Physical

H225	Highly flammable liquid and vapour.

Health

H301	Toxic if swallowed.
H311	Toxic in contact with skin.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H331	Toxic if inhaled.
H335	May cause respiratory irritation.
H350	May cause cancer.

Environmental

H411	Toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P231	Handle under inert gas.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P260	Do not breathe dust/fume/gas/mist/vapours/spray.
P262	Do not get in eyes, on skin, or on clothing.
P270	Do no eat, drink or smoke when using this product.
P272	Contaminated work clothing should not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P284	Wear respiratory protection.

Response

P331	Do NOT induce vomiting.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P370 + P378	In case of fire: Use ... for extinction.

Storage

P405	Store locked up.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.

Disposal

P501	Dispose of contents/container to ...

Figure 14 Hazards

7. GESAMP

Detailed GESAMP profile.

GESAMP Top

GESAMP Hazard profile

A1	A2	B1	B2	C1	C2	C3	D1	D2	D3	E1	E2	E3
2	NR	3	0	2	3	3	2	2	CMSs	NT	DE	3

A1: Bioaccumulation

Rating	Description
2	Low potential to bioaccumulate

A1a:

Rating	Description	Criteria [mg/l]
0	No potential to bioaccumulate	Log Kow < 1

A1b:

Rating	Description	Criteria
2	Low potential to bioaccumulate	10 ≤ BCF < 100

A2: Biodegradation

Rating	Description
NR	Not readily biodegradable

B1: Acute aquatic toxicity

Rating	Description	Criteria [mg/l]
3	Moderately toxic	1 < LC/EC/IC_{50} ≤ 10

B2: Chronic aquatic toxicity

Rating	Description	Criteria [mg/l]
0	Negligible	NOEC > 1

C1: Acute oral toxicity

Rating	Description	Criteria [mg/Kg]
2	Moderate	50 < AOTE ≤ 300

C2: Acute dermal toxicity (skin contact)

Rating	Description	Criteria [mg/Kg]
3	Moderately high	50 < ADTE ≤ 200

C3: Acute inhalation toxicity

Rating	Description	Criteria [mg/l] (4 hours exposure)
3	Moderately high	0.5 < AITE ≤ 2

D1: Skin irritation or corrosion

Rating	Description	Sign	GHS category
2	Irritating	Marked erythema, Obvio	Irritant Category 2

D2: Eye irritation

Rating	Description	Sign	GHS category
2	Irritating	Marked conjunctival hy	Irritant Category 2A

D3: Long-term health effects

Notation	Hazard endpoint	Description	GHS category
C	Carcinogenicity	Chemicals which have been shown to induce or increase the incidence of cancer	Category 1 for Carcinogens
M	Mutagenicity	Cause a permanent change in the amount or structure of genetic material in cells	Categories 1 and 2 for Germ Cell Mutagens
Ss	Skin Sensitization	Cause specific skin hypersensitivity or allergy following skin contact	Category 1 for Skin Sensitizers

E1: Tainting of seafood

Rating	Description
NT	The substance has been tested for tainting and found not to taint following exposure of the fish for 24h to 1mg/l.

E2: Behaviour of chemicals in the marine environment

Rating	Description
DE	Dissolver that evaporates

E3: Interference with the use of coastal amenities

Rating	Interference	Description	Interpretation	Warning
3	Highly objectionable	1 is highly acutely toxic; and/or 2 is severely irritant or corrosive to skin or eyes; and/or 3 is carcinogenic, mutagenic or reprotoxic; and/or 4 is a floater or persistent floater with associated health effects	1 C1 and/or C2 and/or C3 = 4; and/or 2 D1 or D2 = 3, 3A, 3B, or 3C; and/or 3 D3 contains C, M or R; and/or 4 E2 = F or Fp and D3 contains Ss, Sr, T, A, N, or I	Warning issued leading to the closure of amenities

Figure 15 GESAMP

2.2.3 Detailed list of available information

If one parameter is not available, it will not appear is the detailed information page.

1. Description (Figure 10)

Parameter	*Description*
Name	Common name of HNS
CAS number	
UN number	
Chemical formula	
Mixed	"Yes" if HNS is a mix of several chemicals. "No" if not.
Accident occurred	"Yes" if accident reported. "No" if not.
Standard European Behaviour Classification (SEBC)	SEBC code and name
Abilities	Abilities of the HNS
Notable risks	Notable risks
MARPOL Annex II	Category and Description of MARPOL Annex II
GESAMP Hazard profile	Summary of GESAMP profile
Synonyms	List of most common synonyms

2. GHS Security Information (Figure 10)
   Labelling of the HNS according to the Globally Harmonised System of Classification and Labelling of Chemicals (GHS).

3. Physico-chemical properties (Figure 11)

Parameter	*Units*	*Description*
Chemical formula		
Molar mass	g/mol	
Critical molar volume	m^3/mol	
State		State at 25°C and 1 atm
Fusion temperature	°C	
Boiling temperature	°C	
Critical temperature	°C	
Density	Kg/m^3	Density at different value of temperature. (A blue line indicate value determined by CEDRE* in the scope of the project)
Surface tension	mN/m	Surface tension at different value of temperature. (A blue line indicate value determined by CEDRE* in the scope of the project)
Interfacial tension	mN/m	Interfacial tension at different value of temperature.
Kinematic viscosity	cSt	Kinematic viscosity at different value of temperature. (A blue line indicate value determined by CEDRE* in the scope of the project)

Hydrosolubility	mg/l	Hydrosolubility at different value of temperature and salinity. (A blue line indicate value determined by CEDRE* in the scope of the project)
Vapour pressure	Pa	Vapour pressure at different value of temperature.
Critical pressure	Pa	
Vapour pressure at 70% of critical temperature	Pa	
Vapour density		
Flash point (Pensky-Martens closed cup)	°C	
Flash point (Cleveland open cup)	°C	
Lower explosivity limit (LEL)	%	
Upper explosivity limit (UEL)	%	
Vaporization enthalpy	J/Kg	Vaporization enthalpy at different value of temperature.
Combustion enthalpy	J/Kg	
Specific heat capacity	J/(Kg·K)	
Combustion efficiency	%	
Mass flow rate of the combustion surface	Kg/(m^2·s)	
Radiative fraction	%	
Henry's constant	mol/(m^3·Pa)	

*CEDRE : Centre de documentation, de recherche et d'expérimentations sur les pollutions accidentelles des eaux. (http://wwz.cedre.fr/)

4. Behaviour (Figure 12)

Parameter	*Units*	*Description*
Log Kow		Logarithm of the concentration ratio of the test substance in octanol and water. $Log(C_{oct}/C_{water})$
Log Koc		Logarithm of the organic carbon/water partition coefficient.
Hydrolysis (Half-life)	Days	
Aqueous photolysis (Half-life)	Days	
Biodegradation in estuary environment (Half-life)	Days	
Biodegradation in marine environment (Half-life)	Days	
Standard European Behaviour Classification (SEBC)		
Bioconcentration factor (BCF)		

5. Ecotoxicity (Figure 13)

Parameter	*Units*	*Description*
Lowest median lethal concentration (LC_{50}) on algae	mg/l	
Lowest median lethal concentration (LC_{50}) on crustacean	mg/l	
Lowest median lethal concentration (LC_{50}) on fishes	mg/l	
Highest no observed effect concentration (NOEC) on algae	mg/l	
Highest no observed effect concentration (NOEC) on crustacean	mg/l	
Highest no observed effect concentration (NOEC) on fishes	mg/l	
Assessment factor (AF)		Long and short term assessment factor
Predicted No Effect Concentration (PNEC)	µg/l	Long and short term predicted no effect concentration

6. Hazards (Figure 14)
    - Labelling of the HNS according to the Globally Harmonised System of Classification and Labelling of Chemicals (GHS).

    - IDLH

Parameter	*Units*	*Description*
IDLH	ppm	Immediately dangerous to life or health dose

    - A list of hazards (H) and prevention (P) statement according to the Globally Harmonised System of Classification and Labelling of Chemicals (GHS)

7. GESAMP (Figure 15)

    Summarized and detailed GESAMP profile with following columns:
    - **A1 :** Bioaccumulation
        - **A1a**
        - **A1b**
    - **A2 :** Biodegradation
    - **B1 :** Acute aquatic toxicity
    - **B2 :** Chronic aquatic toxicity
    - **C1 :** Acute oral toxicity
    - **C2 :** Acute dermal toxicity (skin contact)
    - **C3 :** Acute inhalation toxicity
    - **D1 :** Skin irritation/corrosion
    - **D2 :** Eye irritation
    - **D3 :** Long-term health effects
    - **E1 :** Tainting of seafood
    - **E2 :** Behaviour of chemicals in the marine environment
    - **E3 :** Interference with the use of coastal amenities

2.3 JSON REST API

The JSON REST API has the same capabilities as the web site search tool, but without user interface and with more advanced search capabilities. It is not dedicated to be used by humans, but by machine. It allow external users to implement their version of the search tool or directly inject HNS parameters in external application (simulation systems, comparison systems, …).

The output format is JSON (JavaScript Object Notation), more information on this format can be found on http://www.json.org/

Example of output : (https://www.hns-ms.eu/api/hns/?limit=1)


```
[
  {
    "id": 1,
    "name": "1,2,6-Trichlorobenzene",
    "cas": "87-61-6",
    "un": 2810,
    "sebc": "S"
  }
]
```

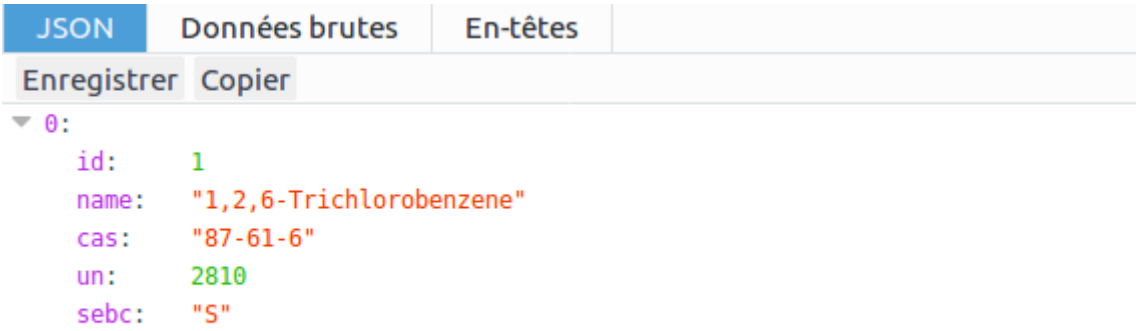



Figure 16 Example of output in a modern web browser

2.3.1 Access

Requirement	Internet connection
URL	https://www.hns-ms.eu/api/hns/

2.3.2 How to use

By default the API return list of the first 20 HNS stored in the database. This output is modified by adding parameters to the URL.

Two type of output are available :

- A list of HNS
- Detailed information about one HNS (only if the “id” parameter is set)

Remarks:

- The first parameter begins with a question mark “?” and the parameters are separated by “&”.
- The order in witch the parameters are added is not important.
- All parameters are optional.

Available parameters:

limit=	*Integer* Sets the maximal number of returned items
offset=	*Integer* Sets the distance from the beginning of the list
order_by=	*[id, name, cas, un, sebc]* Sets the column to order by.
sort=	*[ASC, DESC]* Sets ascending or descending order.
text_search=	*Text* The text field to search. It could be a name a CAS number, UN number or SEBC (space are permitted without quotes)
id=	*Integer* The id of the HNS to get detailed information. If set, all other parameters are ignored.

Examples of usage:

To get the full list of HNS available:

https://www.hns-ms.eu/api/hns/?limit=3000

To get the full list of HNS available sorted by name:

https://www.hns-ms.eu/api/hns/?limit=3000&order_by=name

or

https://www.hns-ms.eu/api/hns/?order_by=name&limit=3000

To get a list of the 2 first HNS containing the word “propane”:

https://www.hns-ms.eu/api/hns/?text_search=propane&limit=2

To get detailed information about the HNS with id=19:

https://www.hns-ms.eu/api/hns/?id=19

Detailed information are only available when the “id” parameter is set. The correspondences between HNS and id are listed in the full list of HNS. The detailed list of available information is presented in Annex 1.

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Registered users tools

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3 Registered users tools

Please note that the full access of HNS-MS Decision-Support System is currently restricted to coastguard operators and response authorities from Belgium, France and other Bonn Agreement contracting parties.

Registered users will get access to the web app (https://www.hns-ms.eu/app/), the place were simulation can be launched and the results viewed.

3.1 Account management

3.1.1 Requesting an account

You may request an account by filling-in the form available at:

https://www.hns-ms.eu/request-account

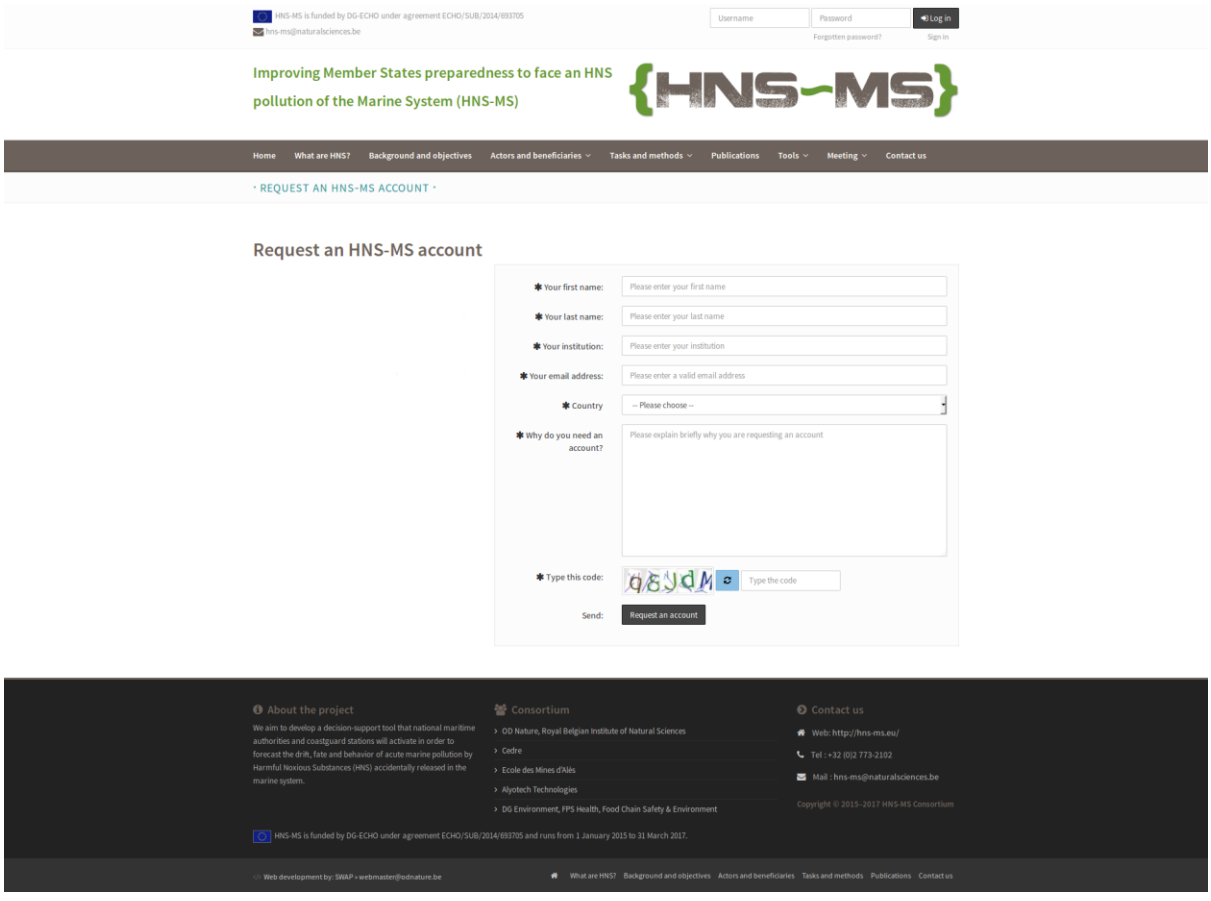


Figure 17 Request an HNS-MS account page

Required information to fill the form:

- Your first and last name
- The name of institution you work in
- A valid email address
- Your country
- Explaining « Why do you need an account? »
- Answering the captcha (Anti-Spam random code)

Processing a new request can take time as an administrator will read and take a decision. You will soon receive an email, just be patient.
In case of acceptance, we strongly recommend you to change your password (Figure 21).

Four type of users are available:

- Administrators

  Users with administration rights.

- Priority users

  Users without administration rights.
  Their simulations have a high level of priority.

- Standard users

  Users without administration rights.
  Their simulations have a normal level of priority.

- Guest users

  Users with view only rights.

3.1.2 Logging in

You may log in by neither using the normal web site top bar (Figure 18) or directly on the web app (Figure 19) using your e-mail address and password.

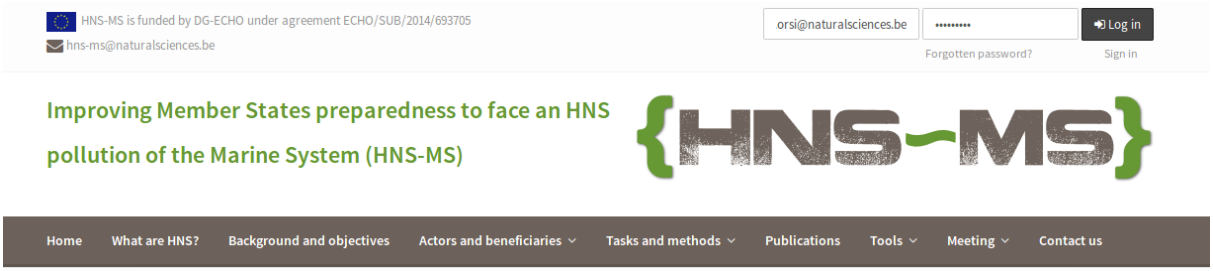


Figure 18 Web site top bar

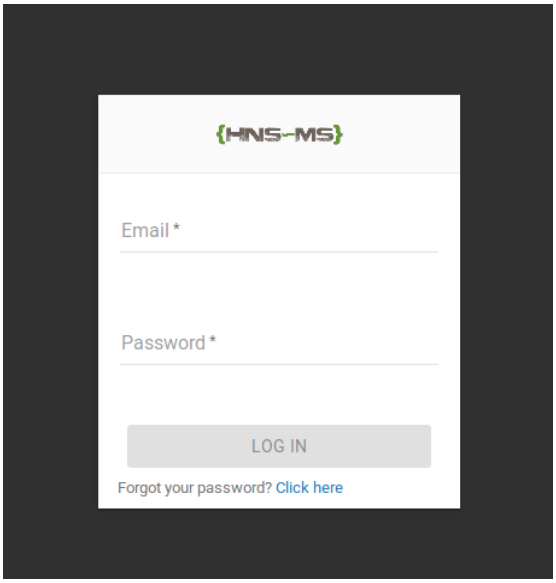


Figure 19 Login form on the web app

3.1.3 User profile and user management

All users can access the user manager at this URL: "https://www.hns-ms.eu/user-manager"

The user manager will act differently to administrators and users.
Users will be able to:

- Edit their own profile by changing the first name, last name, institution name and country. (Figure 20)
- Change their password (Figure 21)

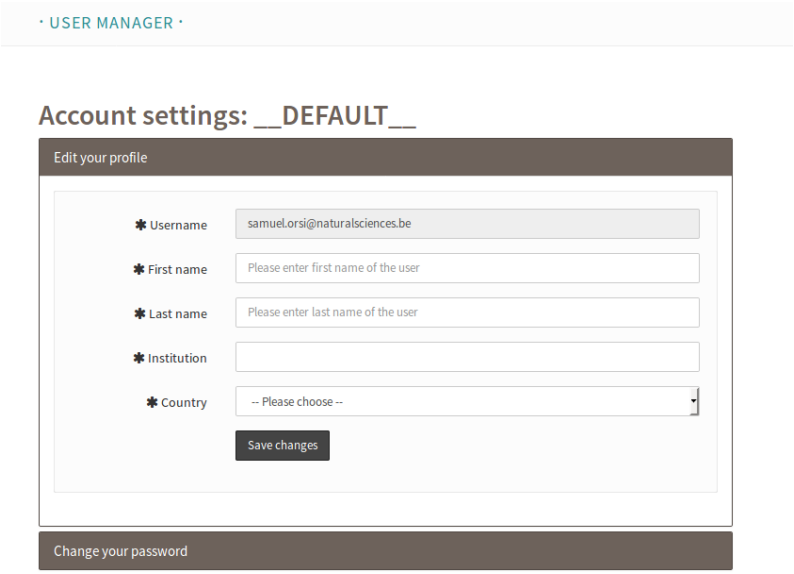


Figure 20 Profile edition

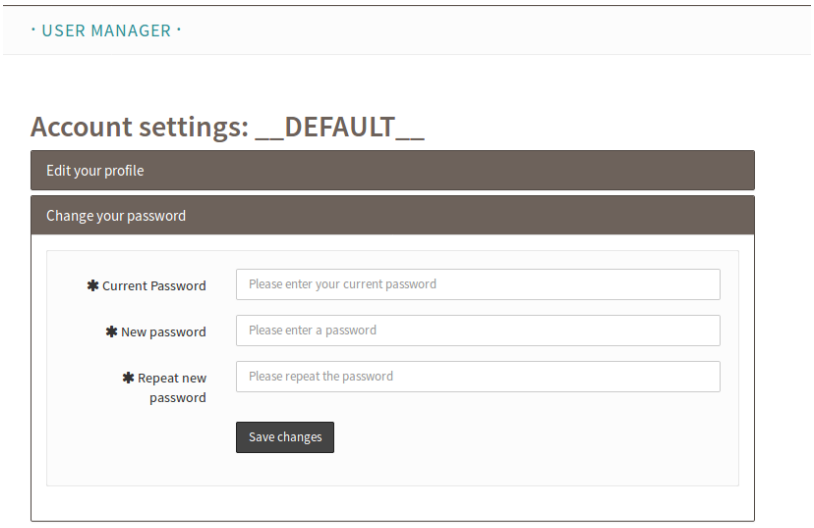


Figure 21 Change password

Administrators will be able to do the same as users, plus:

- User management (Figure 22)
  - Edition of user profile (except administrators)
  - Reset of password
  - Deletion of users (except administrators)
- User creation (Figure 23)

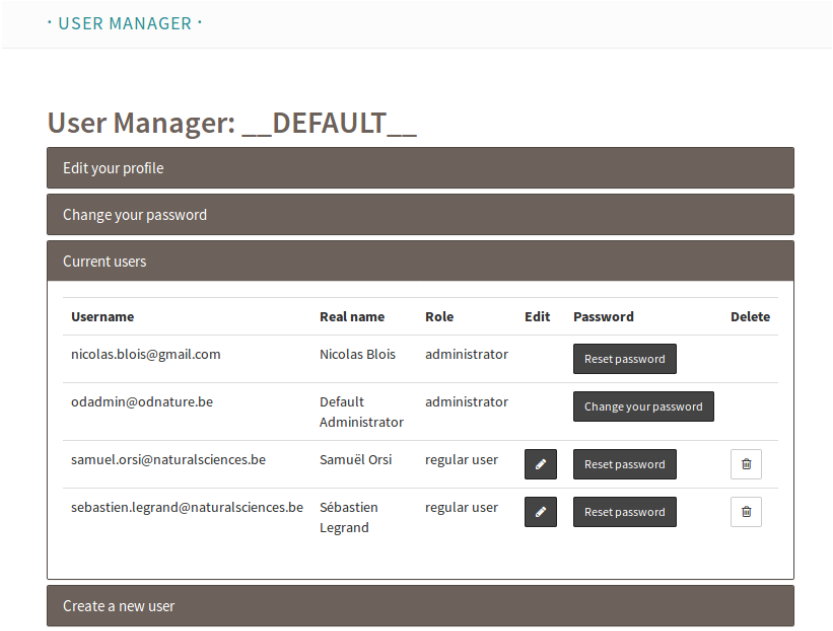


Figure 22 User management

· USER MANAGER ·

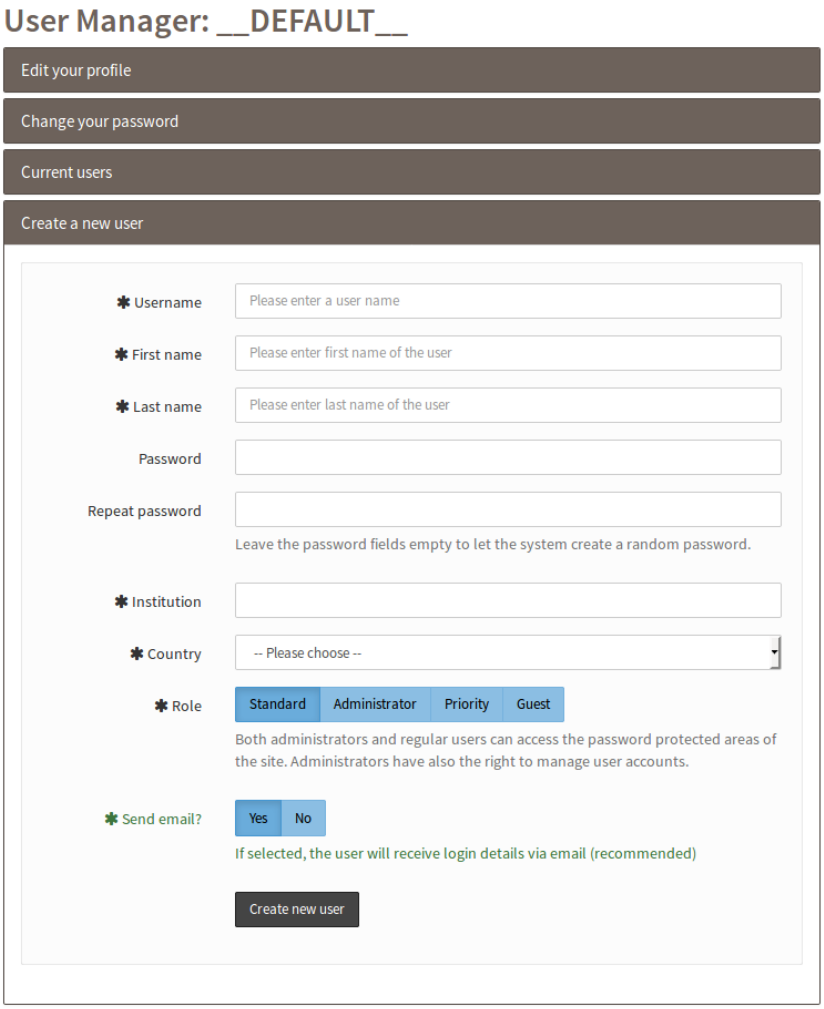


Figure 23 User creation

3.2 HNS-MS decision support system

Remark : This platform is usable on compters with a modern web browser supporting HTML5, CSS3 and JavaScript. It is aloso usable on tablets.

The HNS-MS decision-support system is designed as a web app where users can:

- Create new simulations
- List their simulations as well as those shared by other users.
- View simulation results.
- Search information on HNS in the database.
- Get help to use this app.

Folowing this, the left menu contain :

- New simulation
- My simulations
- Shared simulations
- HNS Database
- Help
- Logout

3.2.1 General navigation

Just after logging in, the user is directed to “My simulation page” (Figure 26).

On the top bar (Figure 24), two buttons are on each side:

- The button on the left side (≡) toggle the left menu
- The button on the right side (⛶) toggle the full screen mode.

Figure 24 The top bar

Figure 25 The left menu

3.2.2 Create a new simulation

On the first logon, the app ask if you want to add a new simulation (Figure 26). You can access to the new simulation page by clicking on the green button or via the left menu (Figure 25).

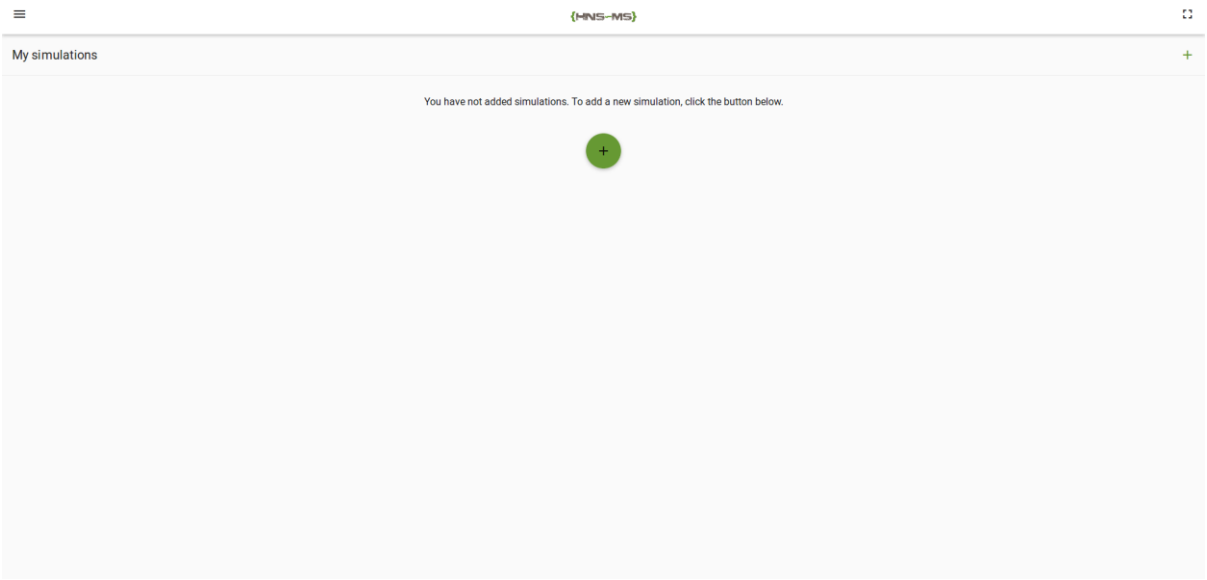


Figure 26 "My simulations" on first login.

The user will access a form were simulation are configured.

By selecting a HNS in the drop down list, physico-chemical parameters will be automatically filled. The user can also override them or enter its own parameters if needed.

A name is required for all new simulation. Please choose wisely!
We recommend at least to use the user name, the involved boat name and scenario type.

Nine HNS spill scenarios will be available:

1. **Observed pollution at sea surface**
    1) Small to medium slick (Surface slick as an ellipsis)

       Backward and forward in time.

       Required parameters:

       – Latitude, longitude of the polluted area
       – Observation time
       – Length, width, orientation of the ellipsis
       – Total HNS volume or thickness of the pollution

    2) Elongated slick (Pollution as a straight line)

       Backward and forward in time

       Required parameters:

       – Latitude, longitude of both end of the pollution
       – Observation time
       – Estimated width of the pollution
       – Total volume of the HNS or slick thickness estimation

2. **Pollution in the water column** (Pollution as an extruded ellipsis)

   Backward and forward in time.

   Required parameters:

   – Latitude, longitude, depth of the polluted water column
   – Observation time
   – Major axis, minor axis, orientation, top and bottom depth
   – Total HNS volume or HNS concentration in the water column

3. **Pollution of the sea floor** (Pollution covers an ellipsis area)

   Backward and forward in time.

   Required parameters:

   – Latitude, longitude, depth of the polluted area
   – Observation time
   – length, width, orientation of the ellipsis
   – Total HNS volume or thickness of the pollution

4. **Release from a moving vessel** (Pollution along a straight line)

   Forward in time only.

   Required parameters:

   - Latitude, longitude at start and end time of the discharge
   - Discharge duration
   - Total HNS volume or discharge rate

5. **Release from a leaking wreck**

   1) Discharge rate estimated

      Only forward in time.

      Required parameters:

      - Latitude, longitude, depth of the wreck
      - Start time of the release
      - End time of the release or release duration
      - Discharge rate [m^3/hr] or total volume released

   2) Discharge rate computed

      Only forward in time.

      Required parameters:

      - Latitude, longitude, depth of the wreck
      - Start time of the release
      - Tank description:
        - Total tank volume & height
        - Total HNS volume
      - Breach description:
        - Number of breaches
        - Height w.r.t. tank bottom
        - Breach diameter

6. **Spill from a broken pipeline**

   Only forward in time.

   Required parameters:

   - Latitude, longitude, depth, diameter, orientation of the breach
   - Start time of the discharge
   - End time of the discharge or discharge duration
   - Discharge volume rate or total HNS volume discharged

7. **Release from a land source or a river**

   Only forward in time.

   Required parameters:

   - Latitude, longitude, depth of the release source
   - Start time of the pollution event
   - End time of the pollution event or duration
   - Total HNS volume spilt or discharge volume rate

8. **Direct gas release in the atmosphere**

   Only forward in time.

   Required parameters:

   1) Latitude, longitude of the source
   2) Start time of the release
   3) End time of the release / duration
   4) Total gas mass (or normalised volume)
   5) Discharge rate

9. **Release from leaking containers adrift**

   Only forward in time.

   This simulation is done in 2 phases:

   1) Simulation of the container trajectory

      Required parameters:

      - Latitude, longitude, time of the cargo loss
      - Number of containers/drums adrift
      - Crosswind and downwind leeway drift coefficient (function of the object adrift and its immerged volume ratio)

   2) Simulation of the HNS drift, fate and behaviour

      Required parameters:

      - HNS volume per container
      - Start time of the release
      - Volume discharge rate

3.2.3 My simulations page

The “My simulations” page (Figure 27) is the first page displayed at logon. It list the simulations owned by the logged user. It is accessible via the left menu (Figure 25).

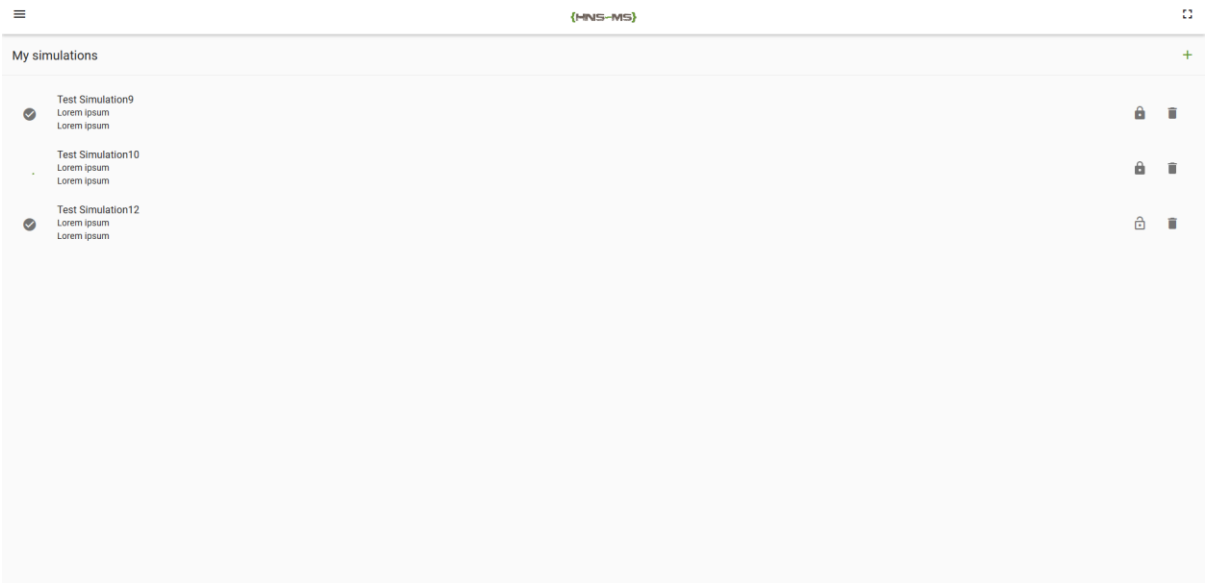


Figure 27 My Simulations

On this pages the user can manage its simulation. As soon at one simulation is created, it will appear on this list.

The icon to the left on each simulation refers to the state of the simulation :

- A running green circle indicate the simulation is pending (waiting for computational power or being in computation)
- A check mark (✓) indicate the results of the simulation are available to view.

Simulation management

On the right of each simulations are control buttons :

- The padlock allow the user to share/unshare its simulation
  (= shared, = private)
- The recycle bin delete a simulation.

3.2.4 Shared simulations page

The “Shared simulations” page (Figure 28) has a similar layout as “My simulations” page, but only list shared simulation between users. Users can only view simulation results. This page is accessible via the left menu (Figure 25).

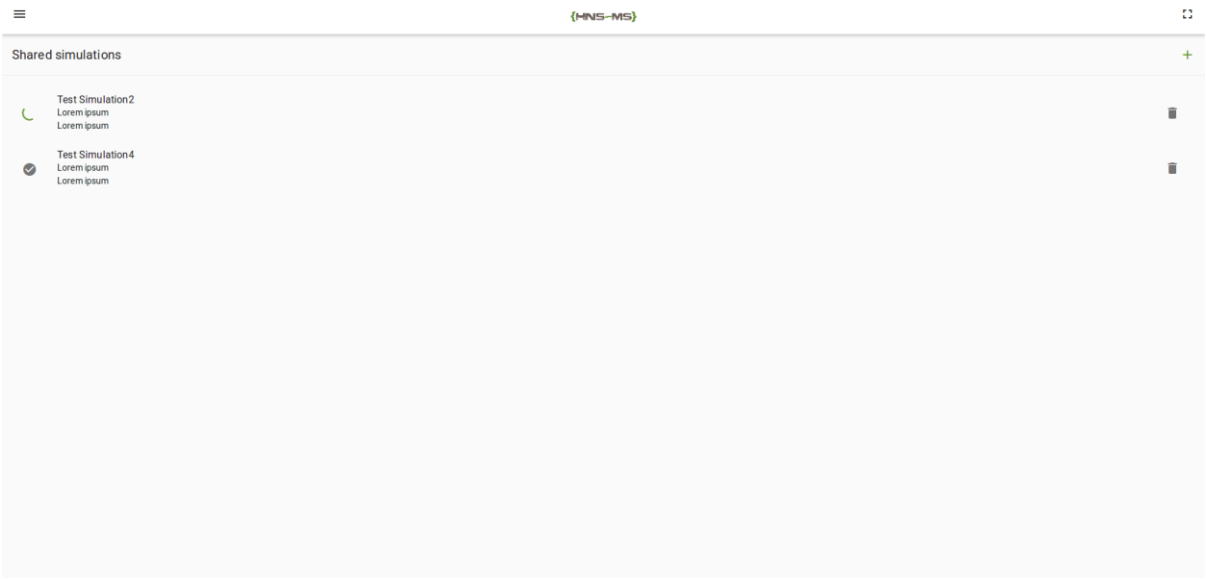


Figure 28 Shared simulations

3.2.5 View simulation results

By clicking on one finished simulation (on the "My simulation page"(Figure 27) or "shared simulations" page(Figure 28)), the users will access the results.

Navigation

The page show at map cantered on the British islands. The users can move the point of view, zoom in and zoom out the map like on any digitalized map.

On the top left is the time (3 - Figure 29). It does not represent the current time, but the time of observation. Exactly like on a typical weather report. Navigation through the time is done by using the controls at the bottom of the page (5 - Figure 29).

At the beginning, the map doesn't show any information, only a regular map. By opening the map menu on the right (4 - Figure 29 and Figure 30) the user can configure the view.

Two tool are visible on the map:

- A measurement tool (1 - Figure 29)
- The current position of the cursor (2 - Figure 29)

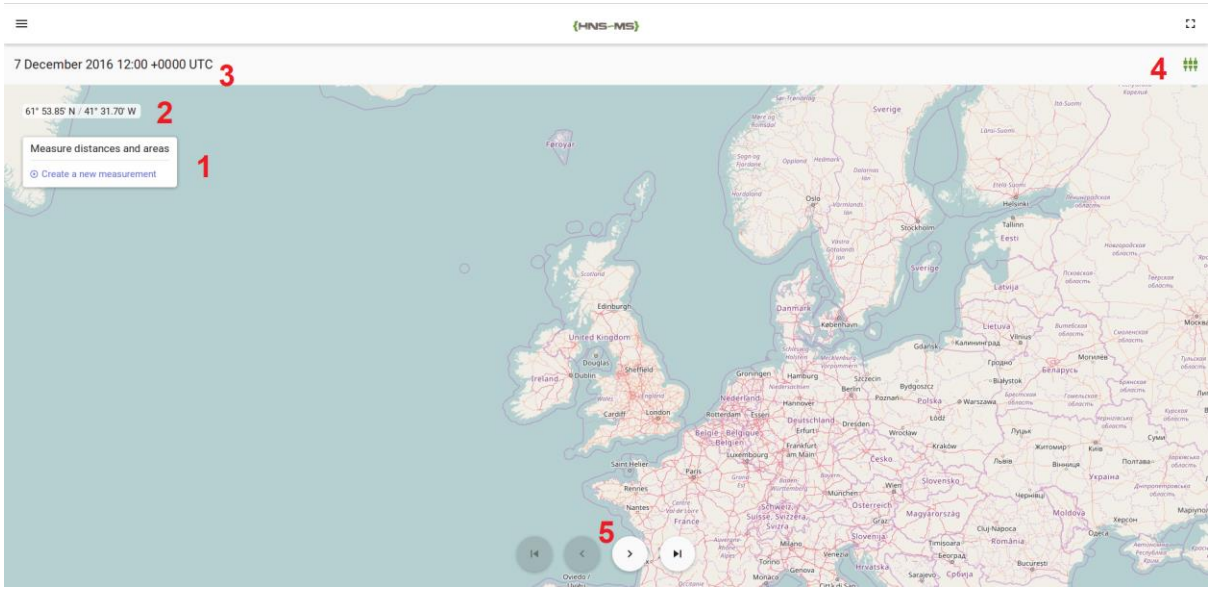


Figure 29 Navigation on the results page

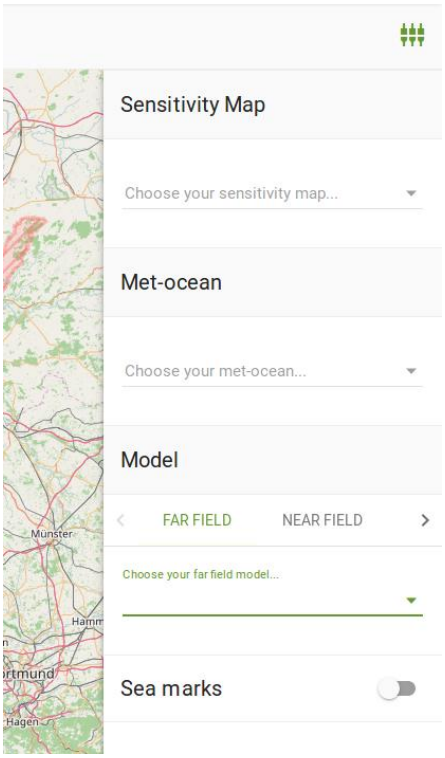


Figure 30 The map menu

Adding a layer on the map

Four layers can be added on the map via the map menu (Figure 30):

- Vulnerability maps (Figure 31)

  Vulnerability maps show the sensitivity of an area. For detail on vulnerability map please refer to page 18.

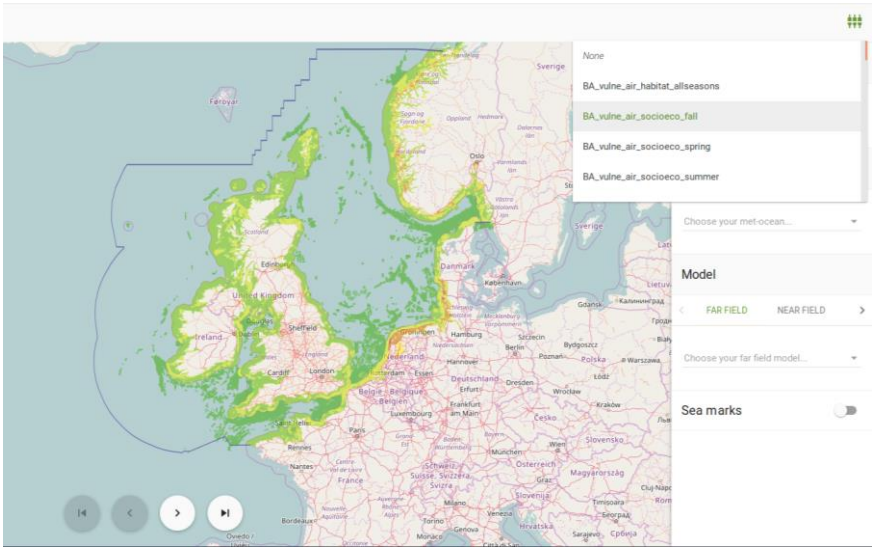


Figure 31 Vulnerability map (scocio-economic - all season)

- Met-oceanic forcing (Figure 32)

  Equivalent to weather prevision but with sea related parameters. It allow users to see the environmental data used by the model.

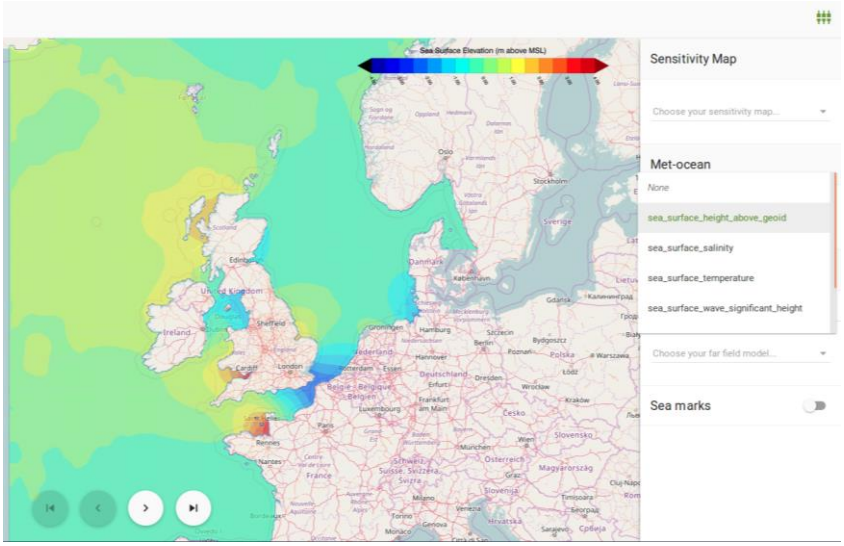


Figure 32 Met-oceanic forcing (Sea surface elevation)

- Results from the model (Figure 33)

  Result from the model showing the evolution of the pollution.

  A model must be selected first :

  - Far field
  - Near field
  - Atmospheric

  Not all models are available at once, it mostly depend on the simulation scenario.

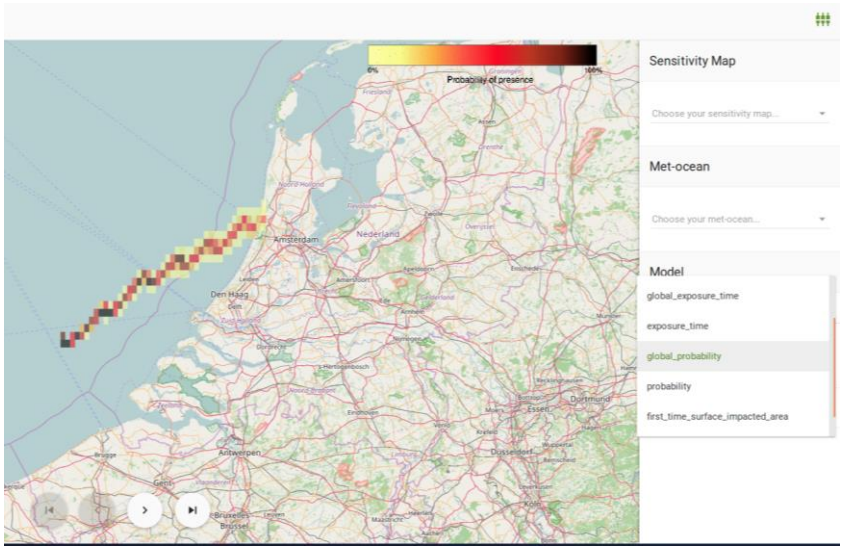


Figure 33 Result from "Far Field model" (probability of presence).

- Sea marks (Figure 34)

  Sea marks from OpenSeaMap is a worldwide open source project.

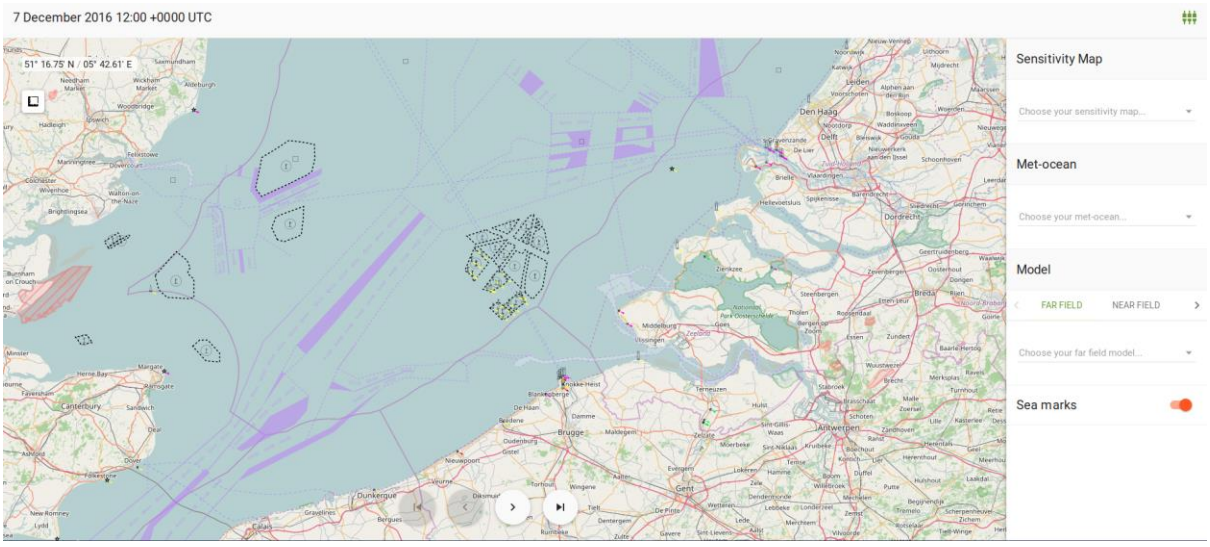


Figure 34 Sea marks from OpenSeaMap

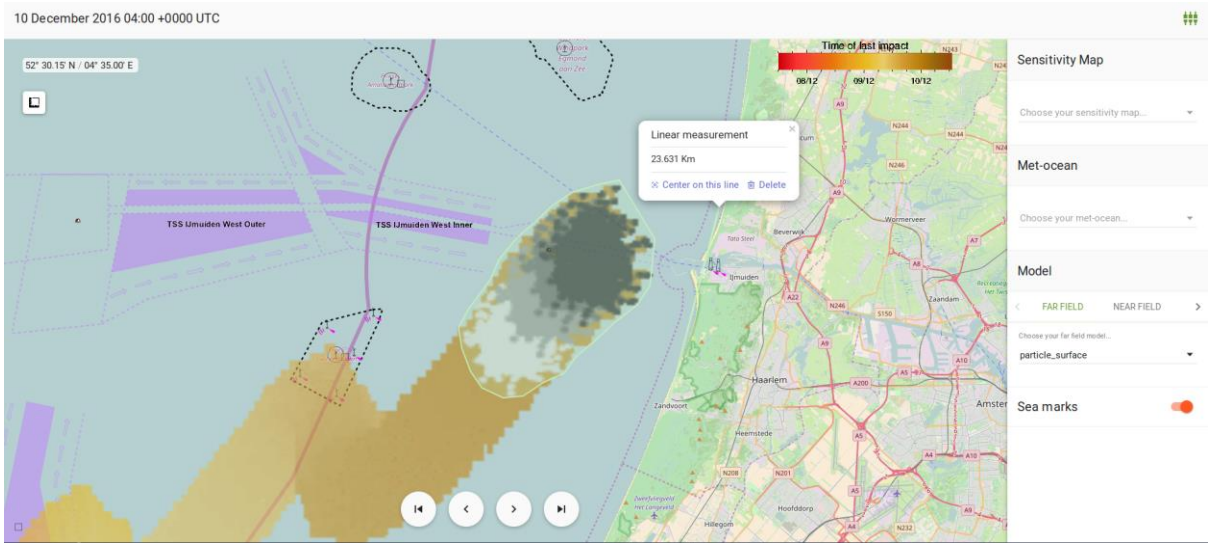
Multiple layers can be used at once to have a better idea of the pollution evolution and impact.

The measurement tool is usable every time.

Example of usage:

Finding the approximate length of coast to protect:
(other methods are possible)

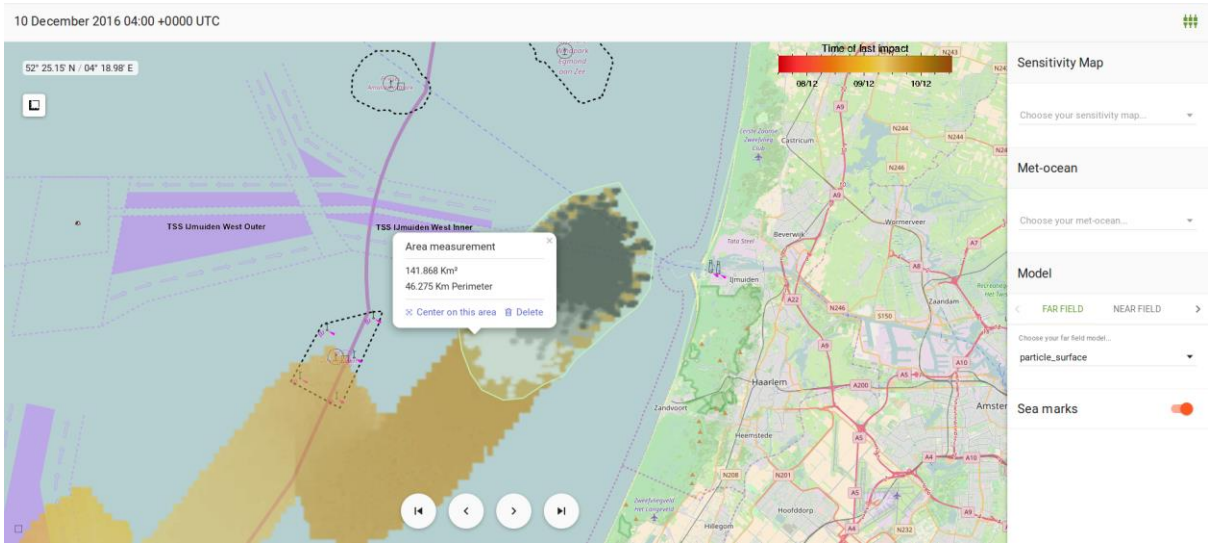
1. Select the model layer “particle_surface”.
2. Navigate in time until the particle are near the coast.
3. Use the measurement tool to determine the approximate length.



Finding the approximate surface covered by the pollution and if it cross navigation routes:

(other methods are possible)

1. Select the model layer “particle_surface”.
2. Turn on Sea marks to view navigation routes
3. Navigate in time until the particle are near the coast.
4. Use the measurement tool to determine the approximate surface covered.



Remarks: As the measurement tool can handle multiple measures. Both of above example can be done together.

3.2.6 HNS-MS database search tool

Chemicals are all different, some make more damages when at sea than on the beach, some exactly the opposite. The purpose of this search tool is to give important information on HNS in terms of toxicity, physical and chemical parameters.

To facilitate access to normal users, scientists or not, an easy to use search tool is provided on the web app.

This tool allow research by four parameters:

- Name (760+ synonyms)
- SEBC Behaviour (floater, dissolver, …)
- CAS Number
- UN Number

Assuming some chemicals could have complex names; the search tool is able to work with a part of it and guide the users to the right substance with the help of a drop down list (Figure 35).
This feature also work with a part of SEBC Behaviour, CAS Number and UN number.

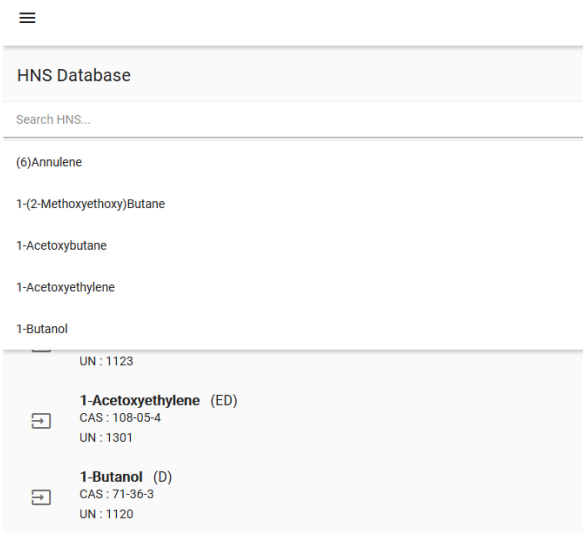


Figure 35 Drop down list

Access

Requirement	Internet connection Modern web-browser
Search tool URL	https://www.hns-ms.eu/app/#/hns/list

The search tool is also accessible on the left menu, by clicking on “HNS Database” (Figure 36).

Figure 36 Where to find the search tool ?

Example of usage:

Let us search information about the chemical having the CAS number “75-86-5” also called “2-Hydroxy-2-Methylpropanenitrile”.

1. Go to the search tool
    a. By direct URL (if already logged in): https://www.hns-ms.eu/app/#/hns/list
    b. Or via the menu bar (see Figure 36) of the web app: https://www.hns-ms.eu/app/

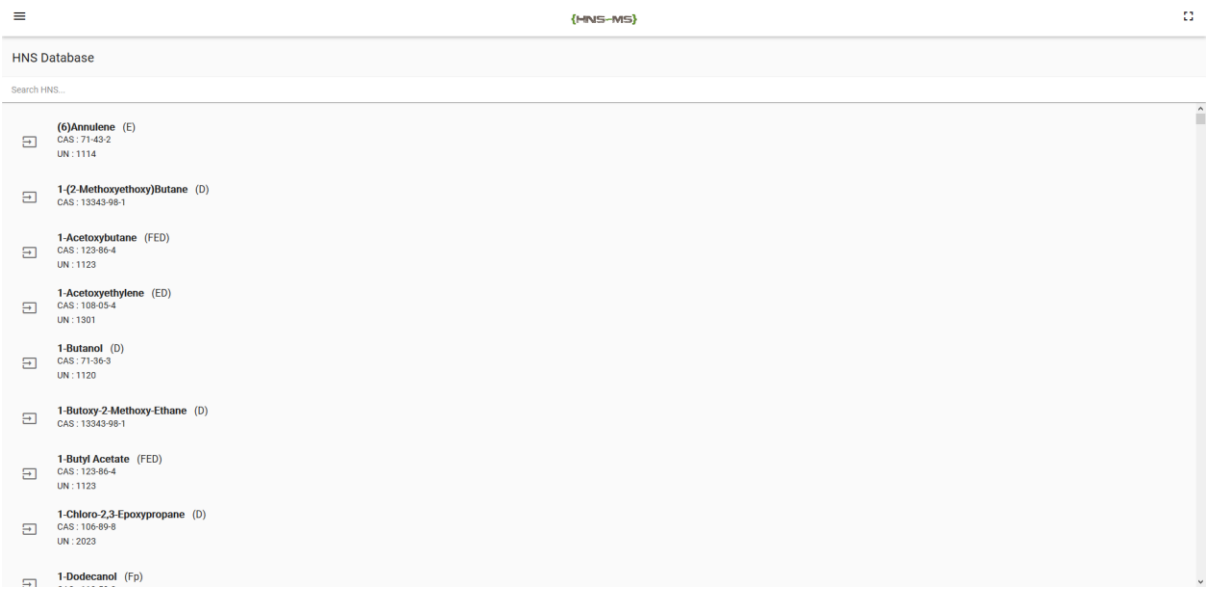


Figure 37 The search tool on the web app

On web app, the search tool displays a complete list of available HNS sorted alphabetically by name. The user can navigate through this list of synonyms to find the targeted chemical. Or use the integrated search tool.

2. In the “Search HNS…” field begin to type “75-86-5”.
   As the user begins to type, a drop down list of 5 HNS appears. More the user will type; more the list will become accurate. The result are sorted by name in alphabetical order.

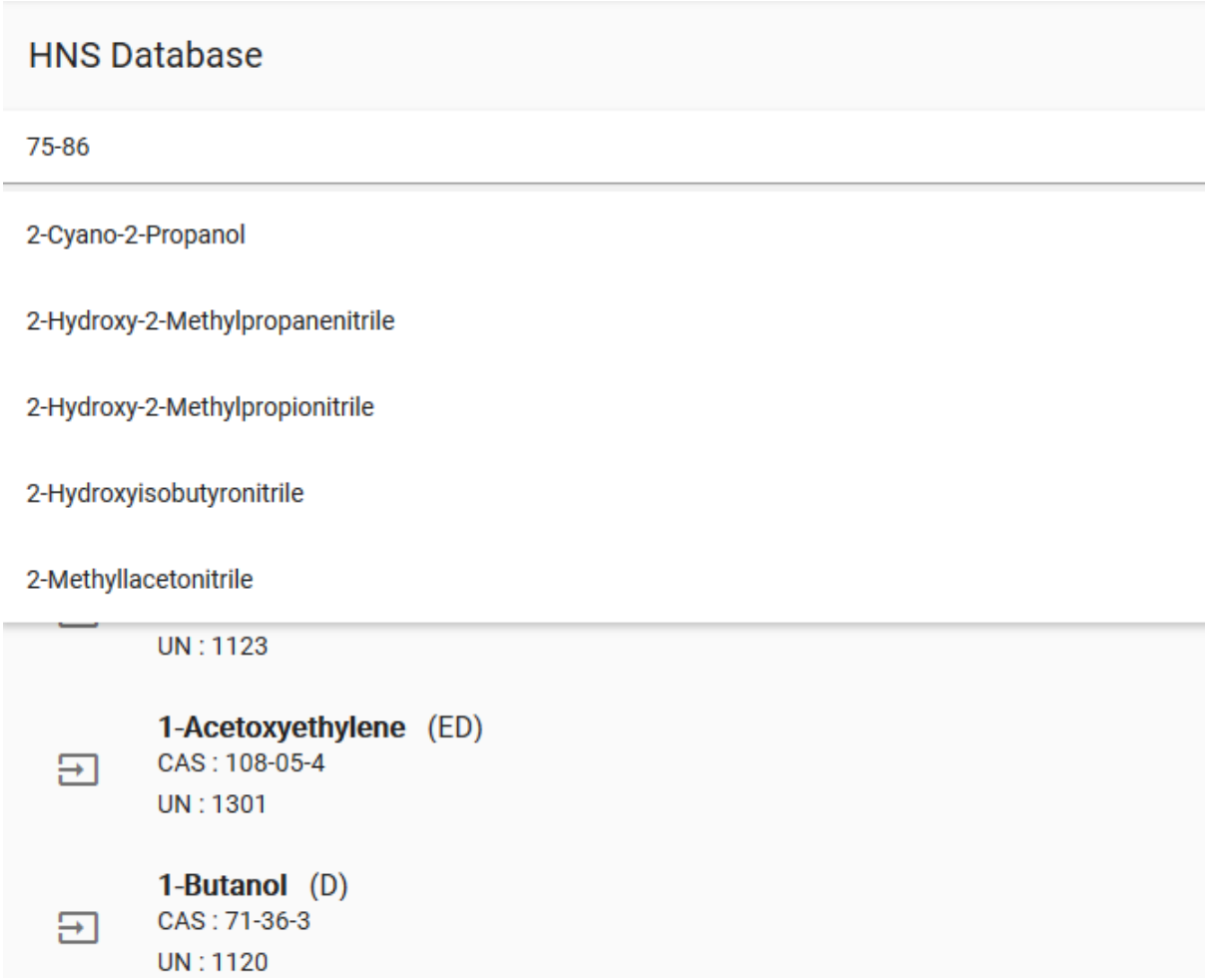


Figure 38 The drop down list under the search field

3. By clicking on one of the chemical listed, the user will access to the detailed information about the HNS.

Detailed information page is described at page 28 of this report “Detailed information page”.

Annex

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Annex 1: Information returned by the HNS-MS JSON REST API

This annex details all the information that can be returned by the HNS-MS JSON REST API presented in section 2.3.

Remark : if the parameter is not available in the database, this parameter will contain the mantion “null”, even in case of large object like an array.

- **id**
  ID of the HNS in the database.
  - Format : Numeric
  - Output exemple :
    `"id": 19`
- **Name**
  Common name of the HNS in the database.
  - Format : Text
  - Output :
    `"Name": "Acrylonitrile"`
- **CAS number**
  CAS number of the HNS.
  - Format : Text
  - Output :
    `"CAS number": "107-13-1"`
- **UN number**
  United Nations number of the HNS
  - Format : Numeric
  - Output exemple :
    `"UN number": 1093`
- **Formula**
  Chemical formula of the HNS
  - Format : Text
  - Output exemple :
    `"Formula": "C3H3N"`
- **Mixed**
  Is the HNS a mix of several chemicals? (“Yes”,”No”, null)
  - Format : Text
  - Output exemple :
    `"Mixed": null`
- **Accident occurred**
  Has the HNS been involved in an accident? (“Yes”,”No”, null)
  - Format : Text
  - Output exemple :
    `"Accident occurred": "Yes"`
- **Abilities**
  Specific abilities of the HNS
  - Format : Text
  - Output exemple :
    `"Abilities ": null`

- **Notable risks**
  Notable risks involved by the HNS
  - Format : Text
  - Output exemple :
    "Notable risks": "Oxidizer. Polymerization."
- **Molar mass**
  Molar mass of the HNS
  - Format : JSON object (vulue, units)
  - Units : g/mol
  - Output exemple :

    ```
    "Molar mass": {
        "value": 53.06,
        "units": "g/mol"
      }
    ```

- **Critical molar volume**
  Critical molar volume of the HNS
  - Format : JSON object (vulue, units)
  - Units : m^3/mol
  - Output exemple :

    ```
    "Critical molar volume": {
        "value": 0.000173,
        "units": "m³/mol"
      }
    ```

- **State at 25 °C and 1 atm**
  State at 25 °C and 1 atm of the HNS
  - Format : Text
  - Output exemple :
    "State at 25 °C and 1 atm": "Liquid"
- **Fusion temperature**
  Fusion temperature of the HNS
  - Format : JSON object (vulue, units)
  - Units : °C
  - Output exemple :

    ```
    "Fusion temperature": {
        "value": -83,
        "units": "°C"
      }
    ```

- **Boiling temperature**
  Boiling temperature of the HNS
  - Format : JSON object (vulue, units)
  - Units : °C
  - Output exemple :

    ```
    "Boiling temperature": {
        "value": 77.4,
        "units": "°C"
      }
    ```


- **Critical temperature**
  Critical temperature of the HNS
  - Format : JSON object (vulue, units)
  - Units : °C
  - Output exemple :

```
"Critical temperature": {
    "value": 540,
    "units": "°C"
  }
```

- **Density**
  Density of the HNS according to the literature. Multiple value by temperature.
  - Format : JSON Array
  - Units : Kg/m^3
  - Output exemple :

```
"Density": [
    {
      "Temperature": {
        "value": 20,
        "units": "°C"
      },
      "value": 810,
      "units": "Kg/m³"
    }
  ]
```

- **Density from CEDRE**
  Density of the HNS taken by CEDRE in the scope on the HNS-MS project. Multiple value by temperature.
  - Format : JSON Array
  - Units : Kg/m^3
  - Output exemple :

```
"Density from CEDRE": null
```

- **Surface tension**
  Surface tension of the HNS according to the literature. Multiple value by temperature.
  - Format : JSON Array
  - Units : mN/m
  - Output exemple :


```
"Surface tension": [
    {
      "Temperature": {
        "value": 20,
        "units": "°C"
      },
      "value": 27.22,
      "units": "mN/m"
    },
    {
      "Temperature": {
        "value": 25,
        "units": "°C"
      },
      "value": 26.63,
      "units": "mN/m"
    }
  ]
```


- **Surface tension from CEDRE**
  Surface tension of the HNS taken by CEDRE in the scope on the HNS-MS project. Multiple value by temperature.
  - Format : JSON Array
  - Units : mN/m
  - Output exemple :


```
"Surface tension from CEDRE": null
```


- **Interfacial tension**
  Interfacial tension of the HNS according to literature. Multiple value by temperature.
  - Format : JSON Array
  - Units : mN/m
  - Output exemple :


```
"Interfacial tension": null
```

- **Kinematic viscosity**
  Kinematic viscosity of the HNS according to the literature. Multiple value by temperature.
  - Format : JSON Array
  - Units : cSt
  - Output exemple :


```
"Kinematic viscosity": [
    {
      "Temperature": {
        "value": 20,
        "units": "°C"
      },
      "value": 0.43,
      "units": "cSt"
    },
    {
      "Temperature": {
        "value": 25,
        "units": "°C"
      },
      "value": 0.42,
      "units": "cSt"
    }
  ]
```


- **Kinematic viscosity from CEDRE**
  Kinematic viscosity of the HNS taken by CEDRE in the scope on the HNS-MS project. Multiple value by temperature.
  - Format : JSON Array
  - Units : cSt
  - Output exemple :


```
"Kinematic viscosity from CEDRE": null
```


- **Hydrosolubility**
  Hydrosolubility of the HNS according to the literature. Multiple value by temperature and salinity.
  - Format : JSON Array
  - Units : mg/l
  - Output exemple :


```
"Hydrosolubility": [
    {
      "Temperature": {
        "value": 20,
        "units": "°C"
      },
      "Salinity": {
        "value": 0,
        "units": "‰"
      },
      "value": 79000,
      "units": "mg/l"
    }
  ]
```

- **Hydrosolubility from CEDRE**
  Hydrosolubility of the HNS taken by CEDRE in the scope on the HNS-MS project. Multiple value by temperature and salinity.
  - Format : JSON Array
  - Units : mg/l
  - Output exemple :
    ```
    "Hydrosolubility from CEDRE": null
    ```
- **Vapour pressure**
  Vapour pressure of the HNS. Multiple value by temperature.
  - Format : JSON Array
  - Units : Pa
  - Output exemple :
    ```
    "Vapour pressure": [
        {
          "Temperature": {
            "value": 20,
            "units": "°C"
          },
          "value": 11500,
          "units": "Pa"
        },
        {
          "Temperature": {
            "value": 25,
            "units": "°C"
          },
          "value": 14470,
          "units": "Pa"
        }
      ]
    ```
- **Critical pressure**
  Critical pressure of the HNS.
  - Format : JSON object (vulue, units)
  - Units : Pa
  - Output exemple :
    ```
    "Critical pressure": {
        "value": 4660000,
        "units": "Pa"
      }
    ```
- **Vapour pressure at 70% of critical temperature**
  Vapour pressure at 70% of critical temperature of the HNS.
  - Format : JSON object (vulue, units)
  - Units : Pa
  - Output exemple :
    ```
    "Vapour pressure at 70% of critical temperature": null
    ```

- **Vapour density**
  Vapour density of the HNS.
  - Format : JSON object (vulue, units)
  - Output exemple :

```
"Vapour density": {
    "value": 1.9,
    "units": ""
  }
```

- **Flash point (Pensky-Martens closed cup)**
  Flash point of the HNS according to Pensky-Martens closed cup method.
  - Format : JSON object (vulue, units)
  - Units : °C
  - Output exemple :

```
"Flash point (Pensky-Martens closed cup)": {
    "value": -1,
    "units": "°C"
  }
```

- **Flash point (Cleveland open cup)**
  Flash point of the HNS according to Cleveland open cup method.
  - Format : JSON object (vulue, units)
  - Units : °C
  - Output exemple :

```
"Flash point (Cleveland open cup)": null
```

- **Upper explosivity limit (UEL)**
  Upper explosivity limit of the HNS.
  - Format : JSON object (vulue, units)
  - Units : %
  - Output exemple :

```
"Upper explosivity limit (UEL)": {
    "value": 17,
    "units": "%"
  }
```

- **Lower explosivity limit (LEL)**
  Lower explosivity limit of the HNS.
  - Format : JSON object (vulue, units)
  - Units : %
  - Output exemple :

```
"Lower explosivity limit (LEL)": {
    "value": 3,
    "units": "%"
  }
```

- **Vaporization enthalpy**
  Vaporization enthalpy of the HNS. Multiple value by temperature.
  - Format : JSON Array
  - Units : J/Kg
  - Output exemple :

```
"Vaporization enthalpy": [
    {
      "Temperature": {
        "value": 77.4,
        "units": "°C"
      },
      "value": 616000,
      "units": "J/Kg"
    }
  ]
```

- **Combustion enthalpy**
  Combustion enthalpy of the HNS.
  - Format : JSON object (vulue, units)
  - Units : J/Kg
  - Output exemple :

```
"Combustion enthalpy": {
    "value": 31900000,
    "units": "J/Kg"
  }
```

- **Specific heat capacity**
  Specific heat capacity of the HNS.
  - Format : JSON object (vulue, units)
  - Units : J/(Kg·K)
  - Output exemple :

```
"Specific heat capacity": {
    "value": 2050,
    "units": "J/(Kg·K)"
  }
```

- **Combustion efficiency**
  Combustion efficiency of the HNS.
  - Format : JSON object (vulue, units)
  - Units : %
  - Output exemple :

```
"Combustion efficiency": {
    "value": 98,
    "units": "%"
  }
```

- **Mass flow rate of the combustion surface**
  Mass flow rate of the combustion surface of the HNS.
  - Format : JSON object (vulue, units)
  - Units : Kg/(m²·s)
  - Output exemple :

```
"Mass flow rate of the combustion surface": {
    "value": 0.05,
    "units": "Kg/(m² ·s)"
  }
```

- **Radiative fraction**
  Radiative fraction of the HNS.
  - Format : JSON object (vulue, units)
  - Units : %
  - Output exemple :

```
"Radiative fraction": {
    "value": 26,
    "units": "%"
  }
```

- **Henry's constant**
  Henry's constant of the HNS.
  - Format : JSON object (vulue, units)
  - Units : mol/(m³·Pa)
  - Output exemple :

```
"Henry's constant": {
    "value": 8.7,
    "units": "mol/(m³ ·Pa)"
  }
```

- **Log Koc**
  Log Koc of the HNS. Logarithm of the concentration ratio of the test substance in octanol and water. Log Koc = $Log(C_{oct}/C_{water})$.
  - Format : JSON object (vulue, units)
  - Output exemple :

```
"Log Koc": {
    "value": -0.07,
    "units": ""
  }
```

- **Log Kow**
  Log Kow of the HNS. Logarithm of the organic carbon/water partition coefficient.
  - Format : JSON object (vulue, units)
  - Output exemple :

```
"Log Kow": {
    "value": -0.92,
    "units": ""
  }
```

- **Hydrolysis (Half-life)**
  Hydrolysis half-life of the HNS.
  - Format : JSON object (vulue, units)
  - Units : days (when hydrolysable)
  - Output exemple :

```
"Hydrolysis (Half-life)": {
    "value": "Not hydrolysable",
    "units": ""
  }
```

- **Aqueous photolysis (Half-life)**
  Aqueous photolysis half-life of the HNS.
  - Format : JSON object (vulue, units)
  - Units : days (when photolysable)
  - Output exemple :

```
"Aqueous photolysis (Half-life)": {
    "value": "Not photolysable",
    "units": ""
  }
```

- **Biodegradation in estuary environment (Half-life)**
  Biodegradation in estuary environment half-life of the HNS.
  - Format : JSON object (vulue, units)
  - Units : days (when biodegradable)
  - Output exemple :

```
"Biodegradation in estuary environment (Half-life)": {
    "value": "Not biodegradable",
    "units": ""
  }
```

- **Biodegradation in marine environment (Half-life)**
  Biodegradation in marine environment half-life of the HNS.
  - Format : JSON object (vulue, units)
  - Units : days (when biodegradable)
  - Output exemple :

```
"Biodegradation in marine environment (Half-life)": {
    "value": "Not biodegradable",
    "units": ""
  }
```

- **Bioconcentration factor (BCF)**
  Bioconcentration factor of the HNS.
  - Format : JSON object (vulue, units)
  - Output exemple :

```
"Bioconcentration factor (BCF)": {
    "value": 1,
    "units": ""
  }
```

- **Lowest median lethal concentration (LC50) on algae**
  Lowest median lethal concentration on algae of the HNS.
  - Format : JSON object (vulue, units)
  - Units : mg/l
  - Output exemple :

```
"Lowest median lethal concentration (LC50) on algae": {
    "value": 1.63,
    "units": "mg/l"
  }
```

- **Lowest median lethal concentration (LC50) on crustacean**
  Lowest median lethal concentration on crustacean of the HNS.
  - Format : JSON object (vulue, units)
  - Units : mg/l
  - Output exemple :

```
"Lowest median lethal concentration (LC50) on crustacean": {
    "value": 6,
    "units": "mg/l"
  }
```

- **Lowest median lethal concentration (LC50) on fishes**
  Lowest median lethal concentration on fishes of the HNS.
  - Format : JSON object (vulue, units)
  - Units : mg/l
  - Output exemple :

```
"Lowest median lethal concentration (LC50) on fishes": {
    "value": 5.16,
    "units": "mg/l"
  }
```

- **Highest no observed effect concentration (NOEC) on algae**
  Highest no observed effect concentration on algae of the HNS.
  - Format : JSON object (vulue, units)
  - Units : mg/l
  - Output exemple :

```
"Highest no observed effect concentration (NOEC) on algae": {
    "value": 0.8,
    "units": "mg/l"
  }
```

- **Highest no observed effect concentration (NOEC) on crustacean**
  Highest no observed effect concentration on crustacean of the HNS.
  - Format : JSON object (vulue, units)
  - Units : mg/l
  - Output exemple :

```
"Highest no observed effect concentration (NOEC) on
crustacean": {
    "value": 0.5,
    "units": "mg/l"
  }
```

- **Highest no observed effect concentration (NOEC) on fishes**
  Highest no observed effect concentration on fishes of the HNS.
  - Format : JSON object (vulue, units)
  - Units : mg/l
  - Output exemple :

```
"Highest no observed effect concentration (NOEC) on fishes": {
    "value": 0.17,
    "units": "mg/l"
  }
```

- **Assessment factor (AF)**
  Assessment factor of the HNS. (Short and long term)
  - Format : JSON Array
  - Output exemple :

```
"Assessment factor (AF)": [
    {
      "value": 100,
      "units": "",
      "Duration": "Short term"
    },
    {
      "value": 100,
      "units": "",
      "Duration": "Long term"
    }
  ]
```

- **Predicted No Effect Concentration (PNEC)**
  Predicted No Effect Concentration of the HNS. (Short and long term)
  - Format : JSON Array
  - Units : µg/l
  - Output exemple :

```
"Predicted No Effect Concentration (PNEC)": [
    {
      "value": 16.3,
      "units": "µg/l",
      "Duration": "Short term"
    },
    {
      "value": 1.7,
      "units": "µg/l",
      "Duration": "Long term"
    }
  ]
```

- **Labelling**
  Labelling names and pictograms of the HNS according to GHS.
  - Format : JSON Array
  - Output exemple :

```
"Labelling": [
    {
      "Name": "Flammable",
      "Symbol": "GHS-SGH02.png"
    },
    {
      "Name": "Corrosive",
      "Symbol": "GHS-SGH05.png"
    },
    {
      "Name": "Toxic",
      "Symbol": "GHS-SGH06.png"
    },
    {
      "Name": "Health Hazard",
      "Symbol": "GHS-SGH08.png"
    },
    {
      "Name": "Environmental Hazard",
      "Symbol": "GHS-SGH09.png"
    }
  ]
```

- **Labelling word**
  Labelling word of the HNS according to GHS. (“Danger”, “Warning” or null)
  - Format : Text
  - Output exemple :

```
"Labelling word": "Danger"
```

- **IDLH**
  Immediately dangerous to life or health dose of the HNS.
  - Format : : JSON object (vulue, units)
  - Units : ppm
  - Output exemple :

```
"IDLH": {
    "value": 85,
    "units": "ppm"
  }
```

- **Standard European Behaviour Classification (SEBC)**
  Standard European Behaviour Classification of the HNS.
  - Format : : Text
  - Output exemple :

```
"Standard European Behaviour Classification (SEBC)": "Dissolver
that evaporates (DE)"
```

- **MARPOL Annex II**
  Classification of the HNS according to the MARPOL Annex II.
  - Format : JSON object (Category, Description)
  - Output exemple :

```
"MARPOL Annex II": {
    "Category": "Y",
    "Description": "Noxious Liquid Substances which, if
discharged into the sea from tank cleaning or deballasting
operations, are deemed to present a hazard to either marine
resources or human health or cause harm to amenities or other
legitimate uses of the sea and therefore justify a limitation
on the quality and quantity of the discharge into the marine
environment."
  }
```

- **Synonyms**
  List of alternate names of the HNS.
  - Format : JSON Array
  - Output exemple :

```
"Synonyms": [
    "Acrylonitrile Monomer",
    "Cyanoethylene",
    "2-Propenenitrile",
    "Propenoic Acid Nitrile",
    "Vinyl Cyanide",
    "Cyanure De Vinyle",
    "Nitrile Acrylique",
    "Acrylonitrile"
  ]
```

- **GESAMP**

  List of GESAMP colums, column names and data of the HNS.

  - Format : JSON Array
  - Output exemple :


```
"GESAMP": [
    {
      "Column": "A1",
      "Name": "Bioaccumulation",
      "Data": {
        "Rating": "2",
        "Description": "Low potential to bioaccumulate"
      }
    },
    {
      "Column": "A1a",
      "Name": null,
      "Data": {
        "Rating": "0",
        "Description": "No potential to bioaccumulate",
        "Criteria": "Log Kow < 1"
      }
    },
    {
      "Column": "A1b",
      "Name": null,
      "Data": {
        "Rating": "2",
        "Description": "Low potential to bioaccumulate",
        "Criteria": "10 ≤ BCF < 100"
      }
    },
    {
      "Column": "A2",
      "Name": "Biodegradation",
      "Data": {
        "Rating": "NR",
        "Description": "Not readily biodegradable"
      }
    },
    {
      "Column": "B1",
      "Name": "Acute aquatic toxicity",
      "Data": {
        "Rating": "3",
        "Description": "Moderately toxic",
        "Criteria": "1 < LC/EC/IC50 ≤ 10"
      }
    },
```

```
{
  "Column": "B2",
  "Name": "Chronic aquatic toxicity",
  "Data": {
    "Rating": "0",
    "Description": "Negligible",
    "Criteria": "NOEC > 1"
  }
},
{
  "Column": "C1",
  "Name": "Acute oral toxicity",
  "Data": {
    "Rating": "2",
    "Description": "Moderate",
    "Criteria": "50 < AOTE ≤ 300"
  }
},
{
  "Column": "C2",
  "Name": "Acute dermal toxicity (skin contact)",
  "Data": {
    "Rating": "3",
    "Description": "Moderately high",
    "Criteria": "50 < ADTE ≤ 200"
  }
},
{
  "Column": "C3",
  "Name": "Acute inhalation toxicity",
  "Data": {
    "Rating": "3",
    "Description": "Moderately high",
    "Criteria": "0.5 < AITE ≤ 2"
  }
},
{
  "Column": "D1",
  "Name": "Skin irritation or corrosion",
  "Data": {
    "Rating": "2",
    "Description": "Irritating",
    "Sign": "Marked erythema, Obvio",
    "GHS category": "Irritant Category 2"
  }
},
```

```
    {
      "Column": "D2",
      "Name": "Eye irritation",
      "Data": {
        "Rating": "2",
        "Description": "Irritating",
        "Sign": "Marked conjunctival hy",
        "GHS category": "Irritant Category 2A"
      }
    },
    {
      "Column": "D3",
      "Name": "Long-term health effects",
      "Data": [
        {
          "Notation": "C",
          "Hazard endpoint": "Carcinogenicity",
          "Description": "Chemicals which have been shown to
induce or increase the incidence of cancer",
          "GHS category": "Category 1 for Carcinogens"
        },
        {
          "Notation": "M",
          "Hazard endpoint": "Mutagenicity",
          "Description": "Cause a permanent change in the
amount or structure of genetic material in cells",
          "GHS category": "Categories 1 and 2 for Germ Cell
Mutagens"
        },
        {
          "Notation": "Ss",
          "Hazard endpoint": "Skin Sensitization",
          "Description": "Cause specific skin hypersensitivity
or allergy following skin contact",
          "GHS category": "Category 1 for Skin Sensitizers"
        }
      ]
    },
    {
      "Column": "E1",
      "Name": "Tainting of seafood",
      "Data": {
        "Rating": "NT",
        "Description": "The substance has been tested for
tainting and found not to taint following exposure of the fish
for 24h to 1mg/l."
      }
    },
```

```
    {
      "Column": "E2",
      "Name": "Behaviour of chemicals in the marine
environment",
      "Data": {
        "Rating": "DE",
        "Description": "Dissolver that evaporates"
      }
    },
    {
      "Column": "E3",
      "Name": "Interference with the use of coastal amenities",
      "Data": {
        "Rating": "3",
        "Interference": "Highly objectionable",
        "Description": "1  is highly acutely toxic; and/or 2
is severely irritant or corrosive to skin or eyes; and/or 3  is
carcinogenic, mutagenic or reprotoxic; and/or 4  is a floater
or persistent floater with associated health effects",
        "Interpretation": "1  C1 and/or C2 and/or C3 = 4;
and/or 2  D1 or D2 = 3, 3A, 3B, or 3C; and/or 3  D3 contains C,
M or R; and/or 4  E2 = F or Fp and D3 contains Ss, Sr, T, A, N,
or I",
        "Warning": "Warning issued leading to the closure of
amenities"
      }
    }
  ]
```

- **Statements**

  List of Hazards (H) and Precautionary (P) statements of the HNS.

  - Format : JSON object
  - Output exemple :


```
"Statements": {
    "Hazards statements": {
      "Physical": [
        {
          "Number": "H225",
          "Statement": "Highly flammable liquid and vapour."
        }
      ],
      "Health": [
        {
          "Number": "H301",
          "Statement": "Toxic if swallowed."
        },
        {
          "Number": "H311",
          "Statement": "Toxic in contact with skin."
        },
        {
          "Number": "H317",
          "Statement": "May cause an allergic skin reaction."
        },
        {
          "Number": "H318",
          "Statement": "Causes serious eye damage."
        },
        {
          "Number": "H331",
          "Statement": "Toxic if inhaled."
        },
        {
          "Number": "H335",
          "Statement": "May cause respiratory irritation."
        },
        {
          "Number": "H350",
          "Statement": "May cause cancer."
        }
      ],
      "Environmental": [
        {
          "Number": "H411",
          "Statement": "Toxic to aquatic life with long lasting
effects."
        }
      ]
    },
```

```
    "Precautionary statements": {
      "Prevention": [
        {
          "Number": "P201",
          "Statement": "Obtain special instructions before
use."
        },
        {
          "Number": "P202",
          "Statement": "Do not handle until all safety
precautions have been read and understood."
        },
        {
          "Number": "P210",
          "Statement": "Keep away from heat/sparks/open
flames/hot surfaces. No smoking."
        },
        {
          "Number": "P231",
          "Statement": "Handle under inert gas."
        },
        {
          "Number": "P242",
          "Statement": "Use only non-sparking tools."
        },
        {
          "Number": "P243",
          "Statement": "Take precautionary measures against
static discharge."
        },
        {
          "Number": "P260",
          "Statement": "Do not breathe
dust/fume/gas/mist/vapours/spray."
        },
        {
          "Number": "P262",
          "Statement": "Do not get in eyes, on skin, or on
clothing."
        },
        {
          "Number": "P270",
          "Statement": "Do no eat, drink or smoke when using
this product."
        },
        {
          "Number": "P272",
          "Statement": "Contaminated work clothing should not
be allowed out of the workplace."
        },
```

```
        {
          "Number": "P273",
          "Statement": "Avoid release to the environment."
        },
        {
          "Number": "P280",
          "Statement": "Wear protective gloves/protective
clothing/eye protection/face protection."
        },
        {
          "Number": "P284",
          "Statement": "Wear respiratory protection."
        }
      ],
      "Response": [
        {
          "Number": "P331",
          "Statement": "Do NOT induce vomiting."
        },
        {
          "Number": "P301 + P310",
          "Statement": "IF SWALLOWED: Immediately call a POISON
CENTER or doctor/physician."
        },
        {
          "Number": "P302 + P352",
          "Statement": "IF ON SKIN: Wash with plenty of soap
and water."
        },
        {
          "Number": "P304 + P340",
          "Statement": "IF INHALED: Remove victim to fresh air
and keep at rest in a position comfortable for breathing."
        },
        {
          "Number": "P305 + P351 + P338",
          "Statement": "IF IN EYES: Rinse cautiously with water
for several minutes. Remove contact lenses, if present and easy
to do. Continue rinsing."
        },
        {
          "Number": "P370 + P378",
          "Statement": "In case of fire: Use ... for
extinction."
        }
      ],
      "Storage": [
        {
          "Number": "P405",
          "Statement": "Store locked up."
        },
```

```
        {
          "Number": "P403 + P233",
          "Statement": "Store in a well-ventilated place. Keep
container tightly closed."
        }
      ],
      "Disposal": [
        {
          "Number": "P501",
          "Statement": "Dispose of contents/container to ..."
        }
      ]
    }
  }
```

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Improving Member States preparedness
to face an HNS pollution of the Marine System