

# A New Framework for Environmental Impact Assessment of HNS: Combining HNS Databases, Population Modelling and Dispersion models

MARINER

**CIIMAR**

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Workshop - Using technology towards a better preparedness to HNS Spills  
**28<sup>th</sup> April 2017 Porto - CIIMAR**





# Actions: Action C.2.3

## C.2.3 Tools for modelling impact (toxicology)

Fate, weathering,  
behaviour and toxicity  
of priority Hazardous  
and Noxious  
Substances



### Physicochemical properties/Characteristics

E	78.114	0.88	12.64
Physical behaviour (GESAMP, 2016)	Molecular Weight (g/mol)	Density (kg/L)	Vapour pressure (KPa; 25°C)
1, 2	2	2	2
5.5	80.1	23.3	
Melting point (°C)	Boiling point (°C)	Volatilization half-life (days)	
2	2	4	

### Substances

Substance name	CAS number	Formulae	Behaviour
1-Dodecanol	112-53-8	C <sub>12</sub> H <sub>26</sub> O	Fp
1-Nonanol	143-08-8	C <sub>9</sub> H <sub>20</sub> O	Fp
1-Nonene	124-11-8	C <sub>9</sub> H <sub>18</sub>	FE
4-Nonylphenol	104-40-5	C <sub>15</sub> H <sub>24</sub> O	Fp
Acrylonitrile	107-13-1	C <sub>3</sub> H <sub>3</sub> N	DE
Aniline	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	FD
Benzene	71-43-2	C <sub>6</sub> H <sub>6</sub>	E
Butyl acrylate	141-32-2	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	FED
Cyclohexane	110-82-7	C <sub>6</sub> H <sub>12</sub>	E
Cyclohexylbenzene	827-52-1	C <sub>12</sub> H <sub>16</sub>	F
Decanoic acid	334-48-5	C <sub>10</sub> H <sub>20</sub> O <sub>2</sub>	Fp
Di-2-ethylhexyl adipate	103-23-1	C <sub>22</sub> H <sub>42</sub> O <sub>4</sub>	Fp
Heptane	142-82-5	C <sub>7</sub> H <sub>16</sub>	E
Hexane	110-54-3	C <sub>6</sub> H <sub>14</sub>	E
Isononanol	27458-94-2	C <sub>9</sub> H <sub>20</sub> O	Fp



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# Actions: Action C.2.3

## C.2.3 Tools for modelling impact (toxicology)

Algae			Invertebrates		
6	EC50	18	Water flea - <i>Daphnia magna</i>		
Parameter 1	Concentration (mg/L)	Species			
Intoxication, immobilization			Freshwater; Static; 20h age		
Endpoint			Observations		
7	EC50	10	Water flea - <i>Daphnia magna</i>		
Parameter 2	Concentration (mg/L)	Species			
Intoxication, immobilization			Freshwater; Static; 20h exposure; Juvenile(s)		
Endpoint			Observations		
8	EC50	10.15	Water flea - <i>Ceriodaphnia dubia</i>		
Parameter 7	Concentration (mg/L)	Species			
Mortality			Freshwater; Static; 25 °C; 24h-exposure; < 24h age		
Endpoint			Observations		
13	LC50	18.4	Water flea - <i>Ceriodaphnia dubia</i>		
Parameter 7	Concentration (mg/L)	Species			
Mortality			Freshwater; Static; 25 °C; 24h-exposure; < 24h age		
Endpoint			Observations		
14	LC50	20	Bay shrimp - <i>Crangon franciscorum</i>		
Parameter 8	Concentration (mg/L)	Species			
Mortality			Saltwater; Static; 16 °C; 96h-exposure; Mature organism(s)		
Endpoint			Observations		
15	LC50	27	Daggerblade grass shrimp - <i>Palaemonetes pugio</i>		
Parameter 9	Concentration (mg/L)	Species			
Mortality			Saltwater; Static; 21 °C; 96h-exposure		
Endpoint			Observations		



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Fate, behaviour and weathering of priority HNS in the marine environment: An online tool



Isabel Cunha <sup>a,1</sup>, Helena Oliveira <sup>a,\*,1</sup>, Teresa Neuparth <sup>a</sup>, Tiago Torres <sup>a</sup>, Miguel Machado Santos <sup>a,b,\*,\*\*</sup>

Fate, weathering, behaviour and toxicity of priority Hazardous and Noxious Substances

**Advanced Search**

Substance name

Behavior at the sea

On this database it is collected information on weathering, behaviour and toxicity of priority Hazardous and Noxious Substances (HNS) from different sources. These systematized information is a useful tool to predict the behaviour of priority HNS in accidental spills and support spill preparedness and effective decision-making process response. This database also provides an important support to risk assessment, environmental impact assessment and monitoring actions.

**Name: 1-Nonene**

CAS Number: 124-11-9

Formula: C<sub>9</sub>H<sub>18</sub>

Physicochemical properties/Characteristics

EF	126.2	0.74	0.72	1.12	0.64
Behavior (EC&AMP, 2016)	Relative Molecular Mass	Density (kg/L)	Vapor pressure (kPa)	Water solubility (mg/L)	Dynamic viscosity (mPa·s)
1, 2	2	2	2	2, 3	2, 3
-81.3	146.9	58.1			
Melting point (°C)	Boiling point (°C)	Vaporization heat (kJ/kg)			
2	2	4			

1. G: Gas; E: Evaporator; F: Floater; Fp: Floater (Particulate); D: Dissolver; S: Sinker

2. Values extracted from the literature and public databases e.g. PubChem

3. "\*" corresponds to values not found in the literature or in available databases

4. Values estimated with models of the EN suite<sup>†††</sup>



1. What? 2. Where? 3. When? 4. Run

Incident Name

2016-10-14 15:27:31 Sim Name

Substance Type

HNS Spill

Chemical Spill Options

- 1-nonanol (Floater)
- Chlorine gas (Gas)
- Ammonia (Gas-Dissolver)
- Benzene (Evaporator)
- Styrene (Evaporator-Floater)
- Di-n-butylamine (Evaporator-Dissolver-Floater)
- Methanol (Evaporator-Dissolver)
- 1-nonanol (Floater)**
- Aniline (Floater-Dissolver)
- Ethanolamine (Dissolver)
- Perchloroethylene (Sinker)

Previous Next



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# CIIMAR HNS database was integrated in MARINER interface.



Name	Behaviour	CAS	Density [kg/m <sup>3</sup> ]	Viscosity [mPa.s]	Solubility [mg/L]	Vapour Pressure [Pa]	Molecular Weight [g/mol]	Log Kow	Source
<input type="checkbox"/> 1-Dodecanol	Floater (Persistent)	112-53-8	830	18.80 at 20°C	4 at 25°C	0.1 at 25°C	186.339	5.13	MARINER (CIIMAR)
<input type="checkbox"/> 1-Nonanol	Floater (Persistent)	143-08-8	830	11.70 at 20°C	140 at 25°C	3 at 25°C	144.258	3.77	MARINER (CIIMAR)
<input type="checkbox"/> 1-Nonene	Evaporator, Floater	124-11-8	740	0.64 at N/D°C	1.12 at 25°C	720 at 25°C	126.243	5.15	MARINER (CIIMAR)
<input type="checkbox"/> 4-Nonylphenol	Floater (Persistent)	104-40-5	950	0.00 at N/D°C	7 at 25°C	0.1 at 25°C	220.356	5.76	MARINER (CIIMAR)



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## Environmental risk assessment

### PNEC

Predicted no-effect concentration

Is the concentration of a substance below which no adverse effects of exposure in an ecosystem are expected to occur, during long-term or short-term exposures.



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## Ecotoxicological dose descriptors

### Chronic toxicity **NOEC** or equivalent **Ec<sub>x</sub>**

- ✓ **Algae** (primary producers): **72/96h EC50** (reproduction/growth);
- ✓ **Invertebrates** (primary consumers): **48h EC50** (immobility) *Daphnia* *sp.* and **96h LC50** other crustaceans;
- ✓ **Fish** (higher level consumers): **96h LC50** (mortality).

The lowest of the availability toxicity values between and within the different trophic levels is used as a toxicological dose descriptor.



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## PNEC<sub>seawater</sub>

Data set	Assessment factor
Lowest short-term L(E)C50 from freshwater or saltwater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels	10,000 <sup>a)</sup>
Lowest short-term L(E)C50 from freshwater or saltwater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels, + two additional marine taxonomic groups (e.g. echinoderms, molluscs)	1000 <sup>b)</sup>
One long-term result (e.g. EC10 or NOEC) (from freshwater or saltwater crustacean reproduction or fish growth studies)	1000 <sup>b)</sup>
Two long-term results (e.g. EC10 or NOEC) from freshwater or saltwater species representing two trophic levels (algae and/or crustaceans and/or fish)	500 <sup>c)</sup>
Lowest long-term results (e.g. EC10 or NOEC) from three freshwater or saltwater species (normally algae and/or crustaceans and/or fish) representing three trophic levels	100 <sup>d)</sup>
Two long-term results (e.g. EC10 or NOEC) from freshwater or saltwater species representing two trophic levels (algae and/or crustaceans and/or fish) + one long-term result from an additional marine taxonomic group (e.g. echinoderms, molluscs)	50
Lowest long-term results (e.g. EC10 or NOEC) from three freshwater or saltwater species (normally algae and/or crustaceans and/or fish) representing three trophic levels + two long-term results from additional marine taxonomic groups (e.g. echinoderms, molluscs)	10

European Chemicals Agency

**PNEC<sub>water, intermittent</sub>: LC(E)50 divided by 100**



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**Layers**

**Vulnerability Index**

- None
- Socio-Economic
- Ecological
- Environmental

**Risk Index**

- Vessel Accident Risk
- Shoreline Contamination Risk (non-modelled)

**User Simulation Layers**

- Zoom to Emission Point

2017-04-25 00:38:36 Sim Name

**Property**

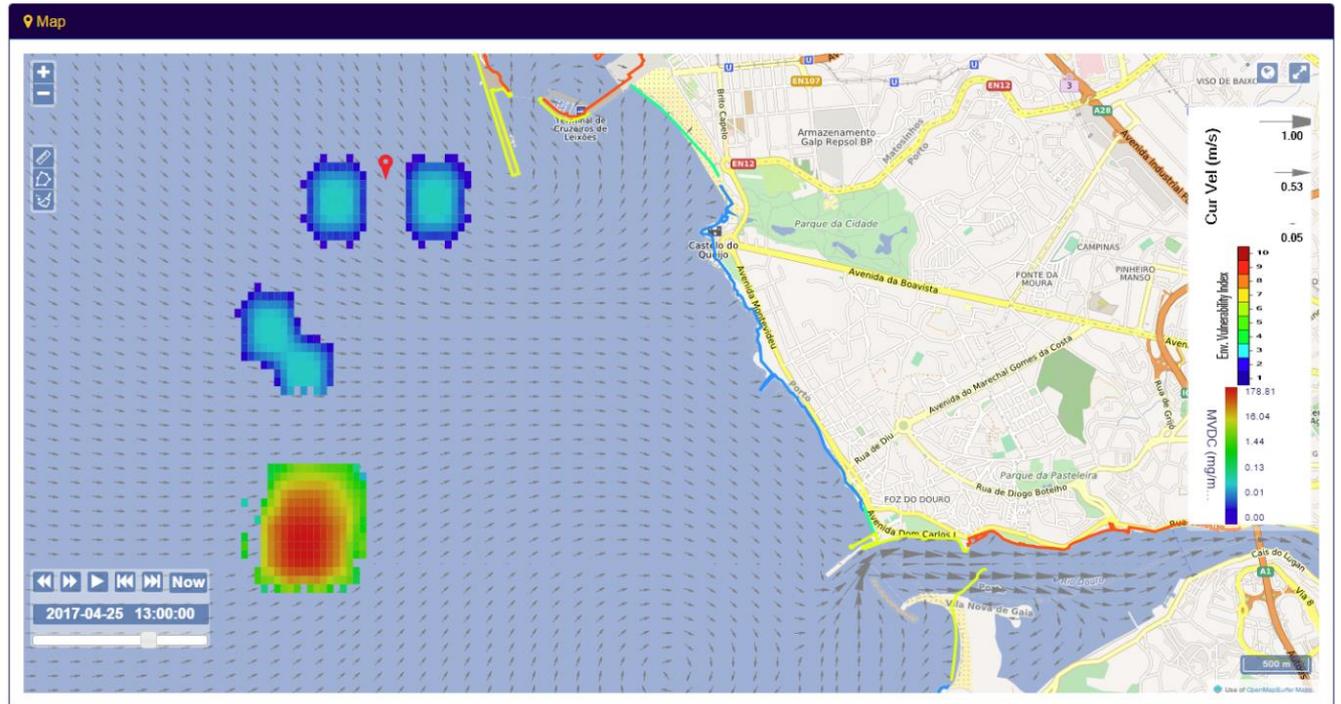
Maximum Vertical Dissolved Concentration [mg/m3]

- Barrier
- Plume Envelope
- Plume Center Trajectory

**General Options**

- Tooltip on Mouse Stop

Export Map





**Layers**

**Domain**  
Portugal (Cont.)

**WMS Layers**

- Vessels
- Monitoring Stations

**Model Results**  
Hydro MOHID AM Douro 50m

- Current Velocity [m/s]
- Current Velocity Modulus [m/s]

**Vulnerability Index**

- None
- Socio-Economic
- Ecological
- Environmental

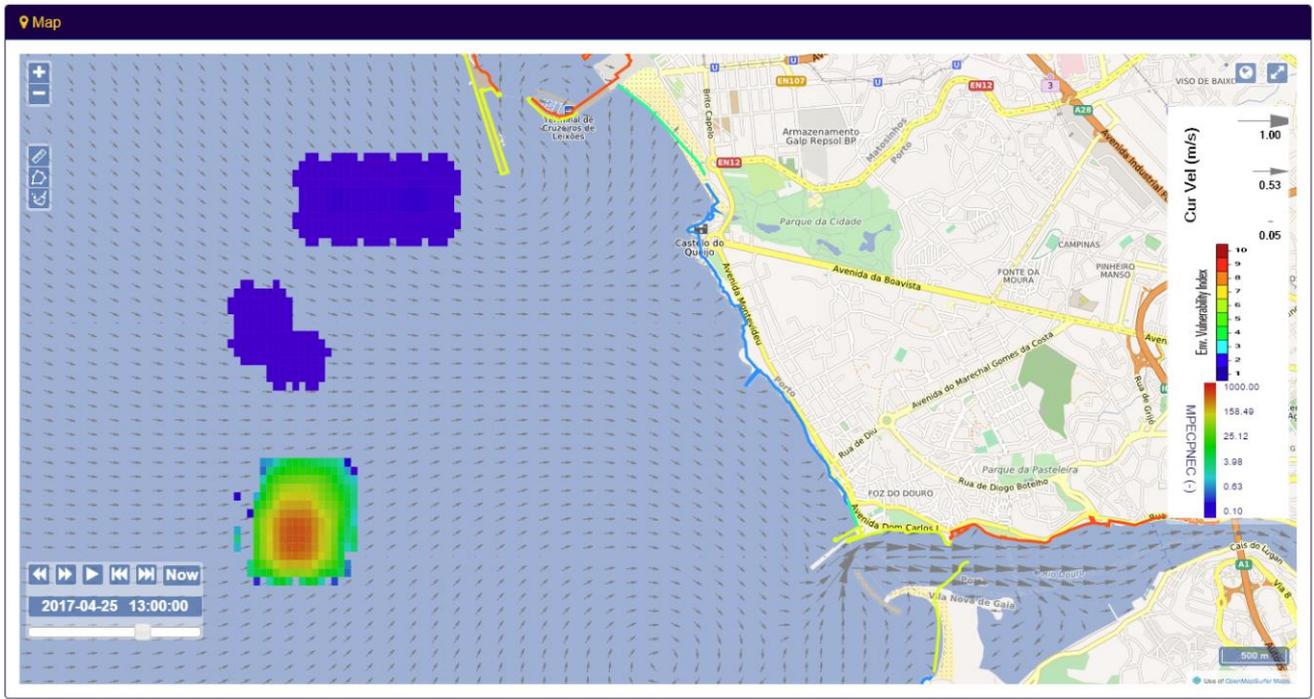
**Risk Index**

- Vessel Accident Risk
- Shoreline Contamination Risk (non-modelled)

**User Simulation Layers**

- Zoom to Emission Point

2017-04-25 00:38:36 Sim Name



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**Layers**

**Vulnerability Index**

- None
- Socio-Economic
- Ecological
- Environmental

**Risk Index**

- Vessel Accident Risk
- Shoreline Contamination Risk (non-modelled)

**User Simulation Layers**

- Zoom to Emission Point

2017-04-25 00:38:36 Sim Name

**Property**

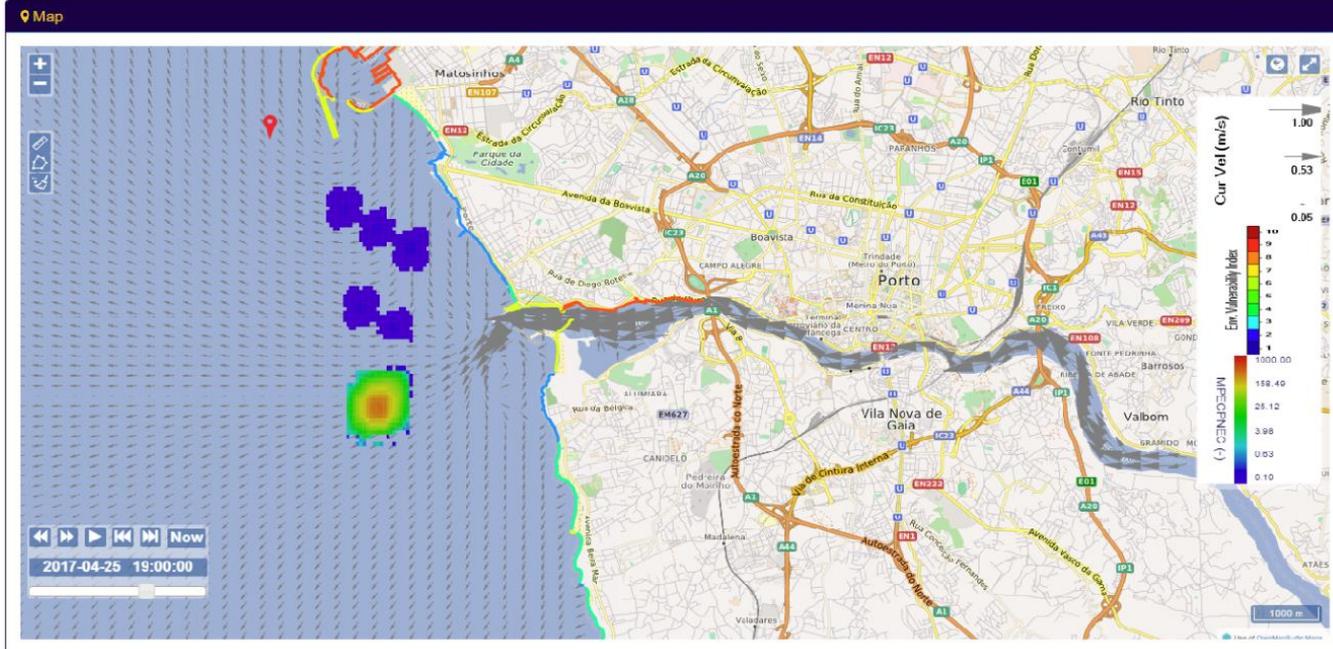
Maximum vertical PEC/PNEC ratio [-]

- Barrier
- Plume Envelope
- Plume Center Trajectory

**General Options**

- Tooltip on Mouse Stop

Export Map



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1. What? 2. Where? 3. When? 4. How

Incident Name: 2016-10-14 15:27:31 Sim Name

Substance Type: HNS Spill

Chemical Spill Options:
 

- 1-Nonane (Flocater)
- Chlorine gas (Gas)
- Ammonia (Gas Dissolver)
- Benzene (Evaporator)
- Styrene (Evaporator/Flocater)
- Du-Substence (Evaporator Dissolver/Flocater)
- Methane (Evaporator Dissolver)
- Aniline (Flocater Dissolver)**
- Chloroacetic Acid (Dissolver)
- Perchloroethylene (Dissolver)

Web Services

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Layers: Vulnerability Index, Risk Index, Use Simulation Layers

Map: 0 Map. Shows a coastal area with a color-coded vulnerability index and a plume trajectory. Legend: 0.06 to 1.00. Date: 2017-04-23 11:00:00

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Aquatic Toxicology 163 (2015) 60–70

Contents lists available at ScienceDirect

**Aquatic Toxicology**

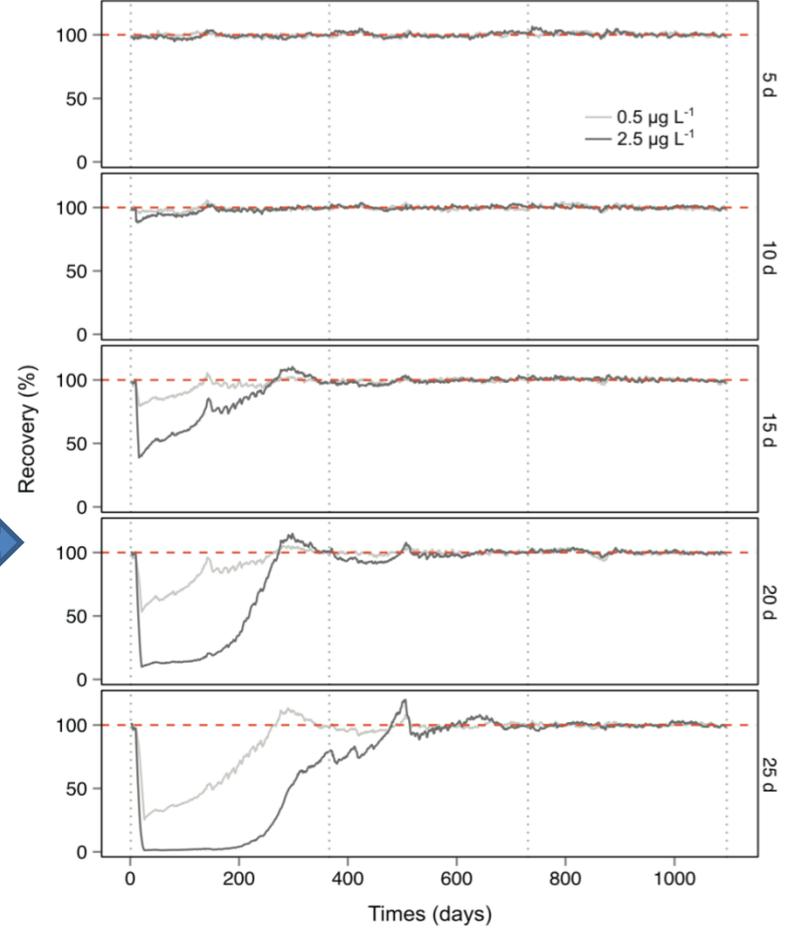
Journal homepage: [www.elsevier.com/locate/aquatox](http://www.elsevier.com/locate/aquatox)

CrossMark



Ecological modelling and toxicity data coupled to assess population recovery of marine amphipod *Gammarus locusta*: Application to disturbance by chronic exposure to aniline

Carmen B. de los Santos<sup>a,\*</sup>, Teresa Neuparth<sup>a</sup>, Tiago Torres<sup>a</sup>, Irene Martins<sup>b</sup>, Isabel Cunha<sup>a</sup>, Dave Sheahan<sup>c</sup>, Tom McGowan<sup>c</sup>, Miguel M. Santos<sup>a,d,e</sup>



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**Thank you**

**Merci**

**Gracias**

**Muito obrigada**

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