





TAKING  
**COOPERATION**  
FORWARD

 online

 *Implementation of modePROCON showcasing for surface water - Po River Basin, Italy*

 boDEREC-CE | Chair of Hydrology and River Basin Management

# OUTLINE

1

Study area

2

Detected  
PPCPs

3

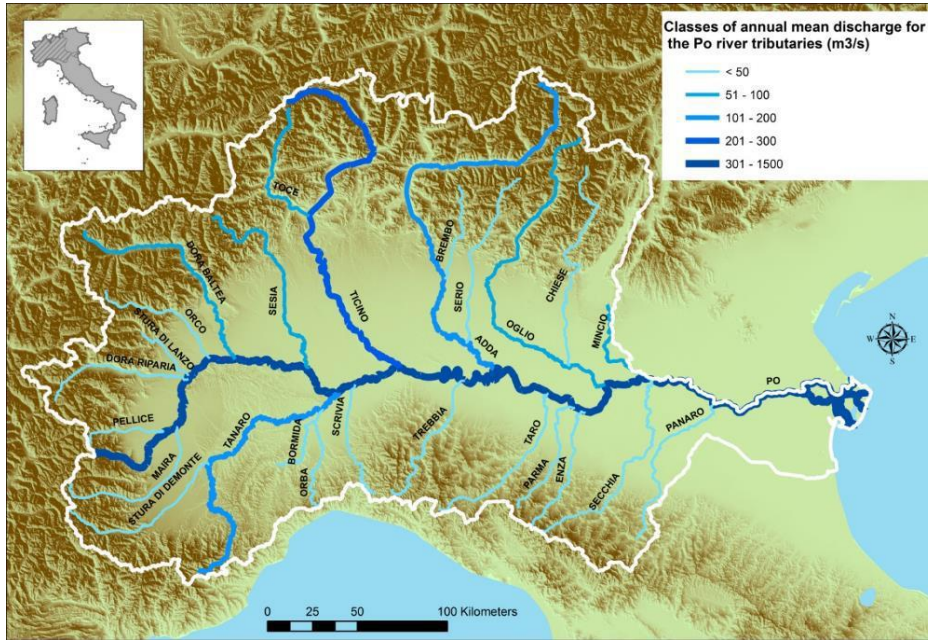
Applying  
modePROCON

4

Model results



# STUDY AREA

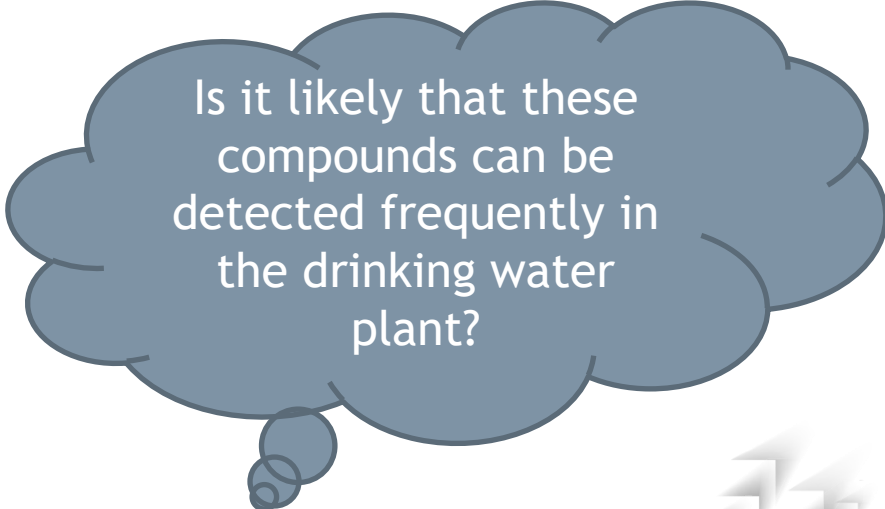


- Investigated drinking water work: Pontelagoscuro
- Po catchment area ~ 774,000 km<sup>2</sup> with 141 rivers and 450 lakes
- Most populated and industrialized basin in Italy
- WWTPs discharging in the river



# DETECTED PPCPs

- The following Emerging Contaminants (ECs) were detected in the influent of the water work Pontelagoscuro:
  - Aminomethylphosphonic acid (AMPA)
  - Iomeprol
  - Diclofenac



Is it likely that these compounds can be detected frequently in the drinking water plant?



# APPLYING modePROCON

## Selecting the water source

PPCP

**Interreg**   
CENTRAL EUROPE European Union  
European Regional  
Development Fund  
**boDEREC-CE**

| <b>Groundwater System</b> | <b>Karst Aquifer System</b> | <b>Surface Water System</b> |
|---------------------------|-----------------------------|-----------------------------|
| <b>Evaluation</b>         | <b>Evaluation</b>           | <b>Evaluation</b>           |
| <b>Model requirements</b> | <b>Model requirements</b>   | <b>Model requirements</b>   |



# APPLYING modePROCON

## Selecting the PPCPs

PPCP

**PPCP Data**

**Units:**

- Solubility: mg/L
- Sorbability (logKow): Unitless
- Volatility (Henry's constant): atI
- Degradability (DT50): Day
- pKa: Unitless

**Data-Reference:**

- [1]: SciFinder
- [2]: CompTox US EPA

|    | Name  | CAS         | Solubility | Sorbability | pKa   | Volatility | Degradability |    |
|----|---|-------------|------------|-------------|-------|------------|---------------|----|
| 55 | <input type="checkbox"/> Ibuprofen-2-hydroxy                    | 51146-55-5  | 13000.0    | 1.68        | 4.44  | 1.92e-09   | 3.11          | Sc |
| 56 | <input type="checkbox"/> Ibuprofen-carboxy                      | 15935-54-3  | 999000.0   | 0.87        | 4.39  | 6.23e-10   | 3.11          | Sc |
| 57 | <input type="checkbox"/> Iohexol                                | 66108-95-0  | 15000.0    | -2.92       | 11.35 | 1.82e-11   | 93.7          | Sc |
| 58 | <input checked="" type="checkbox"/> lomeprol                    | 78649-41-9  | 42000.0    | 2.93        | 11.36 | 1.66e-11   | 95.7          | Sc |
| 59 | <input type="checkbox"/> Iopamidol                              | 60166-93-0  | 8500.0     | -2.55       | 10.87 | 1.72e-11   | 94.7          | Sc |
| 60 | <input type="checkbox"/> Iopromide                              | 73334-07-3  | 160000.0   | -2.66       | 10.62 | 1.43e-11   | 34.9          | Sc |
| 61 | <input type="checkbox"/> Irbesartan                             | 138402-11-6 | 24.0       | 5.25        | 4.16  | 2.85e-09   | 34.8          | Sc |
| 62 | <input type="checkbox"/> Ivermectin                             | 70288-86-7  | nan        | nan         | nan   | nan        | nan           | Sc |
| 63 | <input type="checkbox"/> Keratozin 2-hydroxy-2-hydroxykeratozin | 66014-66-5  | 1300.0     | 0.18        | 10.33 | 1.67e-10   | 31.3          | Sc |

Buttons: Back, Delete all user input, Add new data, Evaluate

- lomeprol and diclofenac are in the provided database.
- AMPA is not contained in the database.
- Thus, it must be added manually.



# APPLYING modePROCON

## Adding a compound to the modePROCON database

PPCP

**Add new data**

**Units:**

- Solubility: mg/L
- Sorbability (logKow): Unitless
- Volatility (Henry's constant): atm\*n
- Degradability (DT50): Day
- pKa: Unitless

Name  CAS

(Entry of CAS Number is optional)

Solubility

Degradability

Sorbability

pKa

Volatility

- The compound's **name**, its **solubility** [mg/L] in water, its **logKow** [-] for the sorbability, its **Henry's law constant** [-] for the volatility, the **DT50** [days] for the biodegradability and the **pKa** [-] are mandatory.



# APPLYING modePROCON

## Adding a compound to the modePROCON database

PPCP

**Add new data**

Name  CAS   
(Entry of CAS Number is optional)

Solubility  Degradability   
Sorbability  pKa   
Volatility

**Units:**

- Solubility: mg/L
- Sorbability (logKow): Unitless
- Volatility (Henry's constant): atm\*n
- Degradability (DT50): Day
- pKa: Unitless

- It is necessary to insert the values in the correct units.
- The new compound will be added to the database by clicking on “Save and Exit”.

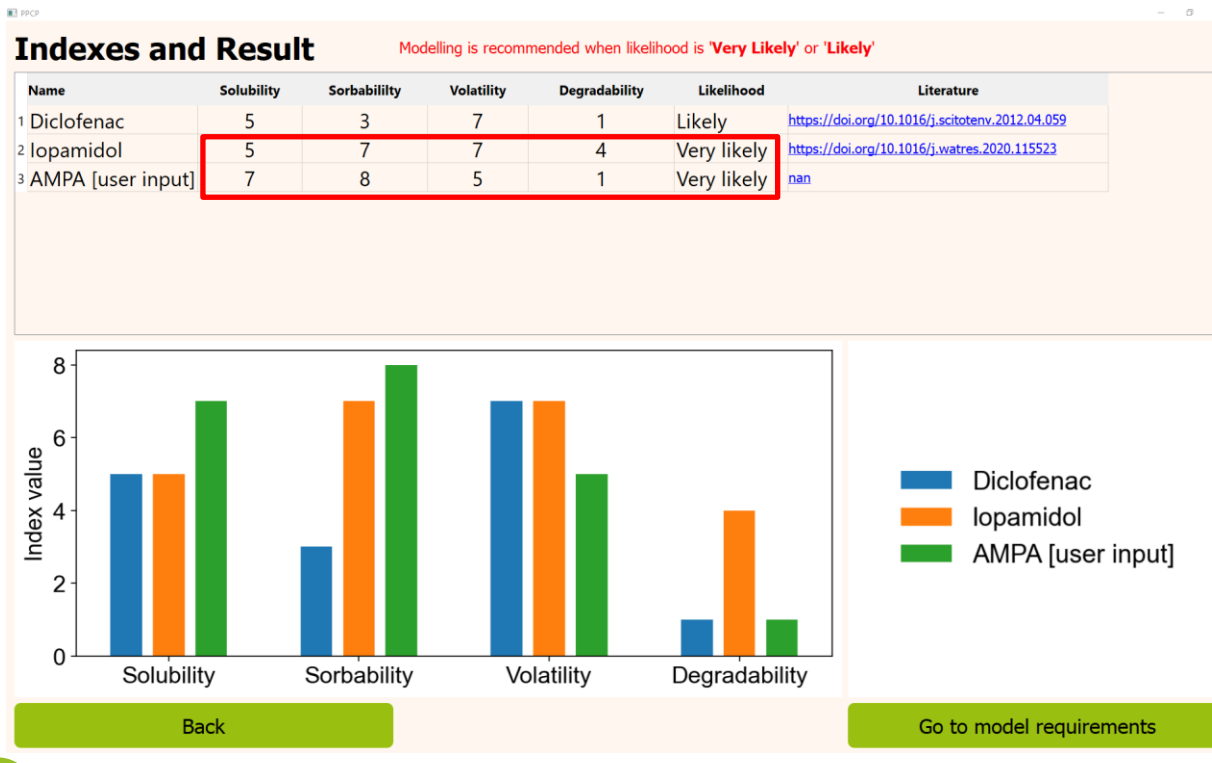
|     |                                     |                            |
|-----|-------------------------------------|----------------------------|
| 113 | <input type="checkbox"/>            | Venlafaxine                |
| 114 | <input type="checkbox"/>            | Verapamil                  |
| 115 | <input type="checkbox"/>            | Warfarin                   |
| 116 | <input type="checkbox"/>            | Test chemical [user input] |
| 117 | <input checked="" type="checkbox"/> | AMPA [user input]          |





# APPLYING modePROCON

## Probability Estimation

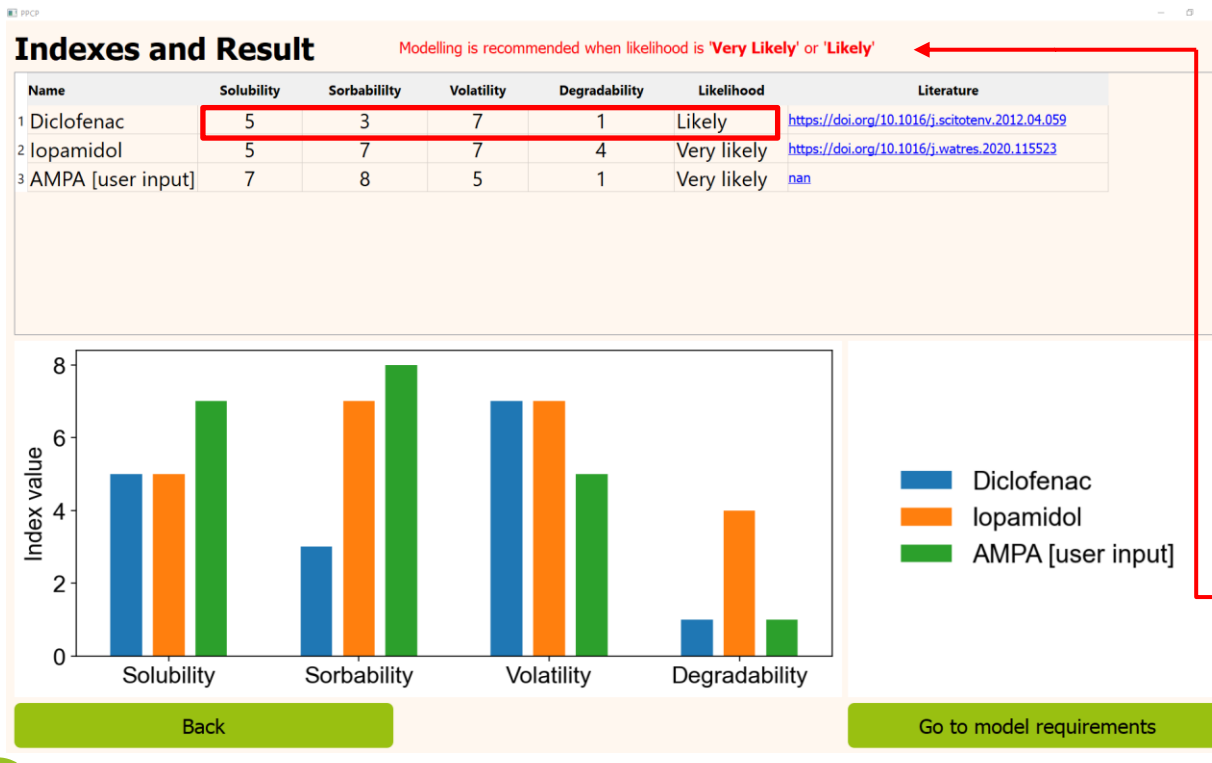


- Although, Iopamidol and AMPA show different values for the considered chemical properties, both compounds can be **very likely** detected in surface water.



# APPLYING modePROCON

## Probability Estimation



- It is likely to detect Diclofenac, as it adsorbs more to organic matter, compared to iomeprol and AMPA.
- modePROCON recommends to model the situation.



# APPLYING modePROCON

## Model requirements

PPCP

### Surface water model requirements

**Evaluate**

Please check the available parameter to evaluate

|   | Parameter   | Application   | Remark |
|---|---|---|--------|
| 5 | <input checked="" type="checkbox"/> Source of contamination       | water.<br>It is needed to set initial conditions for the transport model and define the contaminant source and releases.                        |        |
| 6 | <input type="checkbox"/> Initial concentration of the contaminant | It is needed to set up initial conditions to solve the transport equation and estimate the potential magnitude and impact of the contamination. |        |
| 7 | <input checked="" type="checkbox"/> Point of interest             | Physical locations that are likely to be exposure pathway to come into contact with a contaminated medium.                                      |        |

**Back**

- Except of the upstream inlet concentration of the compounds, the required data is known.
- modePROCON evaluates the data...



# APPLYING modePROCON

## Model requirements

PPCP

### Surface water model requirements

Evaluate

Model cannot be built. Please collect the missing data.

Please check the available parameter to evaluate

|   | Parameter   | Application   | Remark   |
|---|---|---|--|
| 5 | <input checked="" type="checkbox"/> Source of contamination       | water.<br>It is needed to set initial conditions for the transport model and define the contaminant source and releases.                        | The data are available.  |
| 6 | <input type="checkbox"/> Initial concentration of the contaminant | It is needed to set up initial conditions to solve the transport equation and estimate the potential magnitude and impact of the contamination. | It can be estimated by collecting surface water samples from the river. If the source is known, a water sample close to the source is recommended. |
| 7 | <input checked="" type="checkbox"/> Point of interest             | Physical locations that are likely to be exposure pathway to come into contact with a contaminated medium.                                      | The data are available.  |

Back

- ... and replies that a model cannot be built with the available data.
- modePROCON suggests a possibility to obtain the missing data in the remark column.



# APPLYING modePROCON

## Model requirements

PPCP

### Surface water model requirements

**Evaluate**

Model cannot be built. Please collect the missing data.

Please check the available parameter to evaluate

| Parameter   | Application   | Remark   |
|---|---|--|
| <input checked="" type="checkbox"/> 5 Source of contamination       | water.<br>It is needed to set initial conditions for the transport model and define the contaminant source and releases.                        | The data are available.  |
| <input type="checkbox"/> 6 Initial concentration of the contaminant | It is needed to set up initial conditions to solve the transport equation and estimate the potential magnitude and impact of the contamination. | It can be estimated by collecting surface water samples from the river. If the source is known, a water sample close to the source is recommended. |
| <input checked="" type="checkbox"/> 7 Point of interest             | Physical locations that are likely to be exposure pathway to come into contact with a contaminated medium.                                      | The data are available.  |

**Back**

- In this case, AMPA concentrations were available at the inlet.
- A correlation between the AMPA and the PPCPs' concentration was used to estimate a reliable inlet concentration for iomeprol and diclofenac.



# APPLYING modePROCON

## Model requirements

PPCP

### Surface water model requirements

**Evaluate**

It is possible to develop a numerical model. Please communicate with any university or consultant.

Please check the available parameter to evaluate

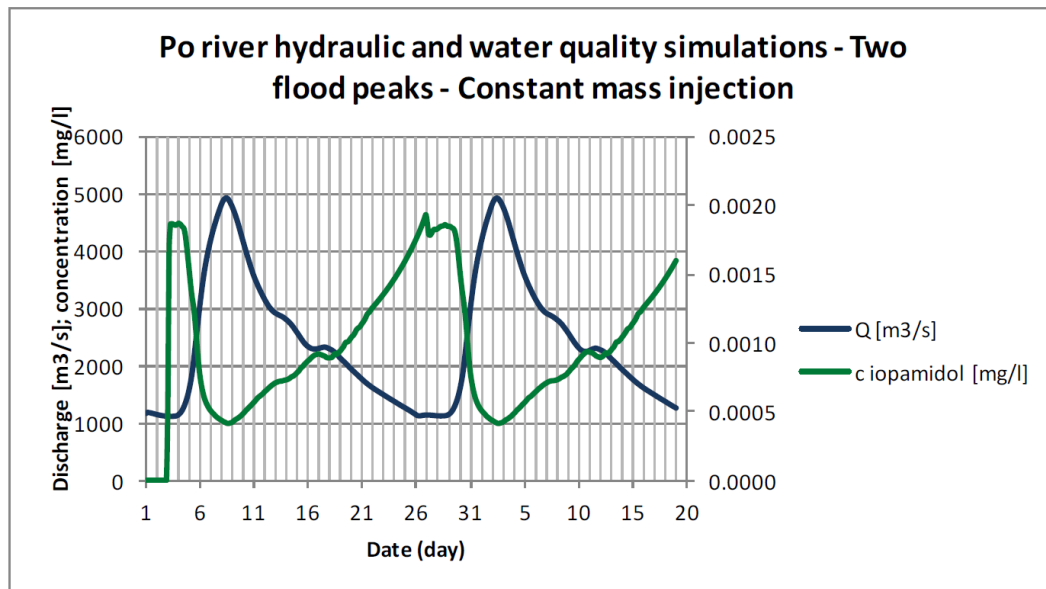
|   | Parameter  | Application   | Remark                  |
|---|--|---|-------------------------|
| 5 | <input checked="" type="checkbox"/> Source of contamination                  | water.<br>It is needed to set initial conditions for the transport model and define the contaminant source and releases.                        | The data are available. |
| 6 | <input checked="" type="checkbox"/> Initial concentration of the contaminant | It is needed to set up initial conditions to solve the transport equation and estimate the potential magnitude and impact of the contamination. | The data are available. |
| 7 | <input checked="" type="checkbox"/> Point of interest                        | Physical locations that are likely to be exposure pathway to come into contact with a contaminated medium.                                      | The data are available. |

**Back**

- With this approach the required information could be obtained.
- modePROCON replies that it is possible to develop a model and the user should communicate with modelling experts.



# MODEL RESULTS



Iopamidol concentration (green) time series in the Po river downstream Panaro confluence compared with the two peaks flow hydrograph (dark blue)

- Indeed, some PPCPs were detected in the influent of the water work Pontelagoscuro.
- Transport modelling is recommended to:
  - assess temporal fluctuations in the PPCPs' concentration
  - estimate maximum concentrations
  - investigate the impact of flow conditions

