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A machine learning model to assess the ecosystem response to water policy measures in the Tagus River Basin (Spain)

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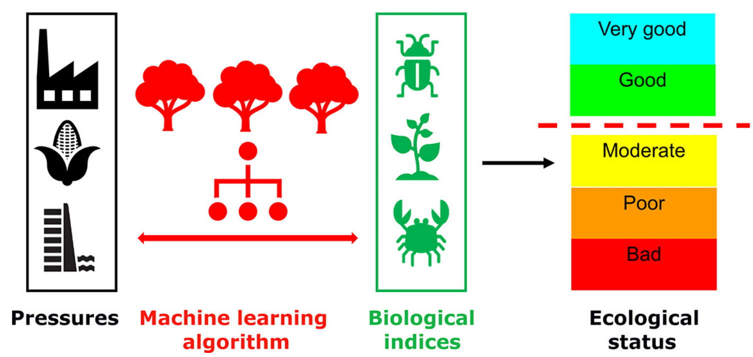
HIGHLIGHTS

- Biological response to multiple stressors was modelled with machine learning.
- Nutrient concentrations and land use showed major effects on biological indices.
- The effect of different nutrient thresholds on the ecosystem was modelled.
- More restrictive nutrient thresholds are needed to comply with the WFD's objectives.
- Improving water and hydromorphology quality would restore the ecosystem status.

GRAPHICAL ABSTRACT



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ABSTRACT

Anthropogenic activities are seriously endangering the conservation of biodiversity worldwide, calling for urgent actions to mitigate their impact on ecosystems. We applied machine learning techniques to predict the response of freshwater ecosystems to multiple anthropogenic pressures, with the goal of informing the definition of water policy targets and management measures to recover and protect aquatic biodiversity. Random Forest and Gradient Boosted Regression Trees algorithms were used for the modelling of the biological indices of macroinvertebrates and diatoms in the Tagus river basin (Spain). Among the anthropogenic stressors considered as explanatory variables, the categories of land cover in the upstream catchment area and the nutrient concentrations showed the highest impact on biological communities. The model was then used to predict the biological response to different nutrient concentrations in river water, with the goal of exploring the effect of different regulatory thresholds on the ecosystem status. Specifically, we considered the maximum nutrient concentrations set by the Spanish legislation, as well as by the legislation of other European Union Member States. According to our model, the current nutrient thresholds in Spain ensure values of biological indices consistent with the good ecological status in only about 60% of the total number of water bodies. By applying more restrictive nutrient concentrations, the number of water bodies with biological indices in good status could increase by almost 40%. Moreover, coupling more restrictive nutrient thresholds with measures that improve the riparian habitat yields up to 85% of water bodies with biological indices in good status, thus proving to be a key approach to restore the status of the ecosystem.

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1. Introduction

Freshwater ecosystems provide vital services to our society, and the maintenance of biodiversity is key to ensure ecosystem productivity and resilience to disturbance (Cardinale et al., 2012; Hooper et al., 2012). Population growth and unsustainable economic development are the main drivers of biodiversity loss (Slingenberg et al., 2009). Rivers are particularly vulnerable to degradation (Palmer and Hondula, 2014), given their crucial role in the human history and being natural recipients of pollutants from the surrounding landscape (Birk, 2019). Multiple anthropogenic pressures, including point and diffuse pollution, alteration of flow regime caused by abstraction or regulation, and hydromorphological degradation are increasingly threatening the health of river ecosystems (Sabater et al., 2019). Climate change is expected to exacerbate the habitat loss (Bussi et al., 2018) and southern Europe will be particularly affected (Füssel et al., 2017). The projected increase in water temperature will lead to a decrease of saturated oxygen and an increase of algal bloom, while the reduction in rainfall expected in some regions will cause an increase in the concentration of contaminants in rivers (Barros et al., 2014). In this context, protecting and restoring riverine ecosystems is a pressing need. Thus, in many countries it is legally required to comply with established environmental targets within specific timeframes (Liao et al., 2018; Volf et al., 2018).

At present, restoration measures aimed at improving ecosystem quality have often proven to be ineffective (Hilderbrand et al., 2005; Voulvoulis et al., 2017). The design of successful strategies for the recovery or maintenance of healthy ecosystems requires understanding the effects of anthropogenic pressures on the biological communities. However, linking pressures to ecological status is a challenging task due to the nonlinear nature of the ecological response (Grizzetti et al., 2017). This becomes even less predictable in situations with multiple stressors. In freshwater ecosystems, anthropogenic stressors originate from a wide range of drivers, including urban and agricultural land use, hydropower generation and climate change (Hering et al., 2010). Hence, considering a single pressure as an isolated driving force in the ecological change is unrealistic and might produce misleading conclusions (Lorenz et al., 2016). Multi-stressor situations require the understanding of the relative importance of each of them (stressor hierarchy, including dominating stressors, reinforcing or mitigation relationships, etc.) and their impacts, in order to find the best combination of mitigation and restoration measures (Lemm et al., 2019). While the literature focusing on ecosystems' behaviour under multiple stressors is growing (see Nõges et al., 2016 for a review), their combined effects are still rarely considered in river basin management (Feld et al., 2016).

In the European Union (EU), the Water Framework Directive (WFD, European Commission, 2000) aims at achieving the "good status" of all water bodies by 2027 at latest. The good status for a surface water body is the result of meeting EU quality standards for specific chemical substances (good chemical status) and having a good ecological status, measured meanly through biological quality elements (BQEs). Thus, with the WFD aquatic ecology gains a key role in water management (Moss, 2008; Hering et al., 2010). The implementation of the Directive, however, is facing challenges (Voulvoulis et al., 2017) and the 2027 deadline is unlikely to be met in all the EU water bodies (Carvalho et al., 2019; European Water Directors, 2019). A major challenge lies in the poorly defined linkages between pressures and their effects on the ecosystem (Carvalho et al., 2019) and, consequently, between pressures and policy measures (Hering et al., 2010). As a matter of fact, the majority (21 out of 28) of Member States did not clearly match pressures and mitigation measures in their Programme of Measures (European Commission, 2015).

More specifically, the WFD requires Member States to establish maximum admissible nutrient concentrations that ensure the achievement of a good ecological status of their surface water bodies (see WFD Annex V, Section 1.2). No further indications on the nutrient thresholds or on the criteria to be used for their quantification are provided by the Directive. Defining nutrient concentration thresholds to ensure the good ecological status is particularly difficult since the processes that determine biological responses to pressures, such as nutrient enrichment, are still not well understood (Dodds et al., 2002; Charles et al., 2019). Member States undertook a process of intercalibration for the BQEs (Poikane et al., 2014) but no intercalibration was required for the physico-chemical supporting elements (Salas Herrero et al., 2019; Bolinches et al., 2020a). This has led to a wide range of nutrient concentration thresholds across EU countries (Laane et al., 2005). In the absence of common guidelines, different methods were used by national authorities to set standards, e.g. expert judgment, establishing a percentile of the distribution of nutrient concentrations in all the water bodies or in the water bodies classified as good, or applying regression between nutrients and biological response (Poikane et al., 2019). In this complex context, the effectiveness of the current nutrient thresholds in supporting the ecological status has been questioned (Carvalho et al., 2019).

Different approaches have been employed to quantify the impact of stressors on the ecosystem (see Sabater et al., 2019 for a review). In recent years, machine learning has shown its potential for the understanding and prediction of ecological phenomena (Olden et al., 2008), especially in complex ecosystems where traditional techniques of analysis could fail. Advanced machine learning methods can model complex and nonlinear relationships without the restrictions typical of parametric approaches (Olden and Jackson, 2002), even if the models are generally more difficult to interpret (Prasad et al., 2006). Several machine learning algorithms have been tested to explore pressures-ecosystem relationships, such as: Artificial Neural Network (Gebler et al., 2017), Multi Target Stepwise Model Tree Induction (Volf et al., 2018), Logistic Regression and Model Trees (Holguin-Gonzalez et al., 2013), Random Forest (Liao et al., 2018), or Gradient Boosted Regression Trees (Hain et al., 2018; Zajicek et al., 2018). By applying these algorithms, a wide range of riverine studies have been investigated. Data-driven ecological models have been used to predict the biological response to mitigation measures. For example, Holguin-Gonzalez et al. (2013) assessed the effect of different wastewater management scenarios on macroinvertebrates, while Olaya-Marín et al. (2012) evaluated how measures of hydromorphological improvement affect the fish species richness. Lynch et al. (2018) and Steel et al. (2018) investigated flow-ecology relationships to understand how to define environmental flows able to restore ecosystem integrity. Other authors successfully estimated the habitat suitability of biological communities in rivers (e.g. Vezza et al., 2015; Muñoz-Mas et al., 2018). Moreover, the literature reports several examples of machine learning ecological models addressing the effects of climate and socio-economic scenarios on biological communities (e.g. Hain et al., 2018; Herrero et al., 2018; Stefanidis et al., 2018).

Setting adequate regulatory targets is of key importance to reach specific environmental objectives (Moldan et al., 2012). To our knowledge, however, the application of machine learning for this purpose is still limited. Phillips et al. (2019) applied regression and categorical statistical methods on synthetic datasets in the case of one or two stressors to assess nutrient targets, but finding satisfactory solutions in case of multiple pressures is still an open challenge (Phillips et al., 2018). Our study aims at contributing to this body of literature by developing a machine learning model to predict the potential effectiveness of water policy targets in a multiple stressors system, the Tagus Basin (central Spain), with a special focus on nutrient concentration thresholds in surface water bodies.

Two machine learning algorithms - Random Forest (RF) (Breiman, 2001) and Gradient Boosted Regression Trees (GBRT) (Friedman, 2001) - were used to establish linkages between anthropogenic stressors on river stretches and the status of freshwater biological elements. The response variable in the model was the biological status expressed by the biological indices of two BQEs (macroinvertebrates and diatoms). The stressors (explanatory variables) belong to the following categories: physicochemical water quality, land use, alteration of the hydrological regime and hydromorphological degradation. The performance of RF and GBRT algorithms was compared and the stressors were ranked according to their predictive power. The obtained model was used to evaluate the effect of current and potential policy measures on the status of the ecosystem. In particular, the response of biological indices to the maximum nutrient concentrations established by the Spanish legislation was modelled to identify hotspots where those nutrient thresholds could be inefficient to reach the WFD objectives. The effect of setting more restrictive nutrient boundaries and improving the quality of the riparian habitat was also modelled. The ultimate goal was to determine the optimal conditions supporting the good ecological status in all the water bodies of the studied river basin and to define additional actions for the recovery of the most degraded river stretches.

To our knowledge, this study is the first analysis quantifying pressures-ecosystem relations in the Tagus river basin. Given the critical water quality issues in the basin especially in the river stretches directly downstream of the Madrid metropolitan region (see Cubillo et al., 1992; Paredes et al., 2010; Bolinches et al., 2020b), our study sheds light on the assessment of the relative importance of stressors and their impacts under different scenarios, hoping to inform future water management decisions. There is evidence that these case-specific approaches are the best alternative for situations with multiple stressors (Schinegger et al., 2018). This study shows how such analysis can provide a useful guide to the definition of policy targets in multiple stressors contexts, depending on the site-specific conditions. The same approach could be applied to any water body where a similar dataset is available. We focused on the biological response to nutrient values, since setting the nutrient threshold that ensure the good status is still an unsolved issue in the context of the WFD.

2. Materials and methods

2.1. Study area

The Tagus is the longest river in the Iberian Peninsula, stretching over 1092 km (Fig. 1). Its basin covers an area of 83,680 km^2, of which 66.5% belongs to Spain and the remaining 33.5% to Portugal. The Central System to the north, the Iberian System to the east and the Montes de Toledo to the south delimit the Spanish part of the catchment area. The central part of the basin consists in a depression originated during the Alpine Orogeny and filled with Cenozoic materials (sands, clays, marls, gypsum and some limestone in the upper levels). Older geological materials (Pre-Cambrian, Palaeozoic and Mesozoic) characterize the borders of the catchment. The vast extension of the basin along the east-west axis results in a significant variability in elevation, climate and geology, leading to a heterogeneous landscape. The climate is Mediterranean with continental features. Annual average temperatures are irregularly distributed within the catchment, ranging from 8°C in the mountain peaks in the north to 17°C in the western area. The average annual precipitation is 648 mm, with a high variability with respect to season and elevation. The heterogeneity of the landscape is reflected in the high asymmetry of the network of tributaries of the Tagus River, with abundant discharge in the right tributaries and short watercourses and low discharge in the left ones. It is the most populated basin in Spain with almost 8 million inhabitants, mainly concentrated in the

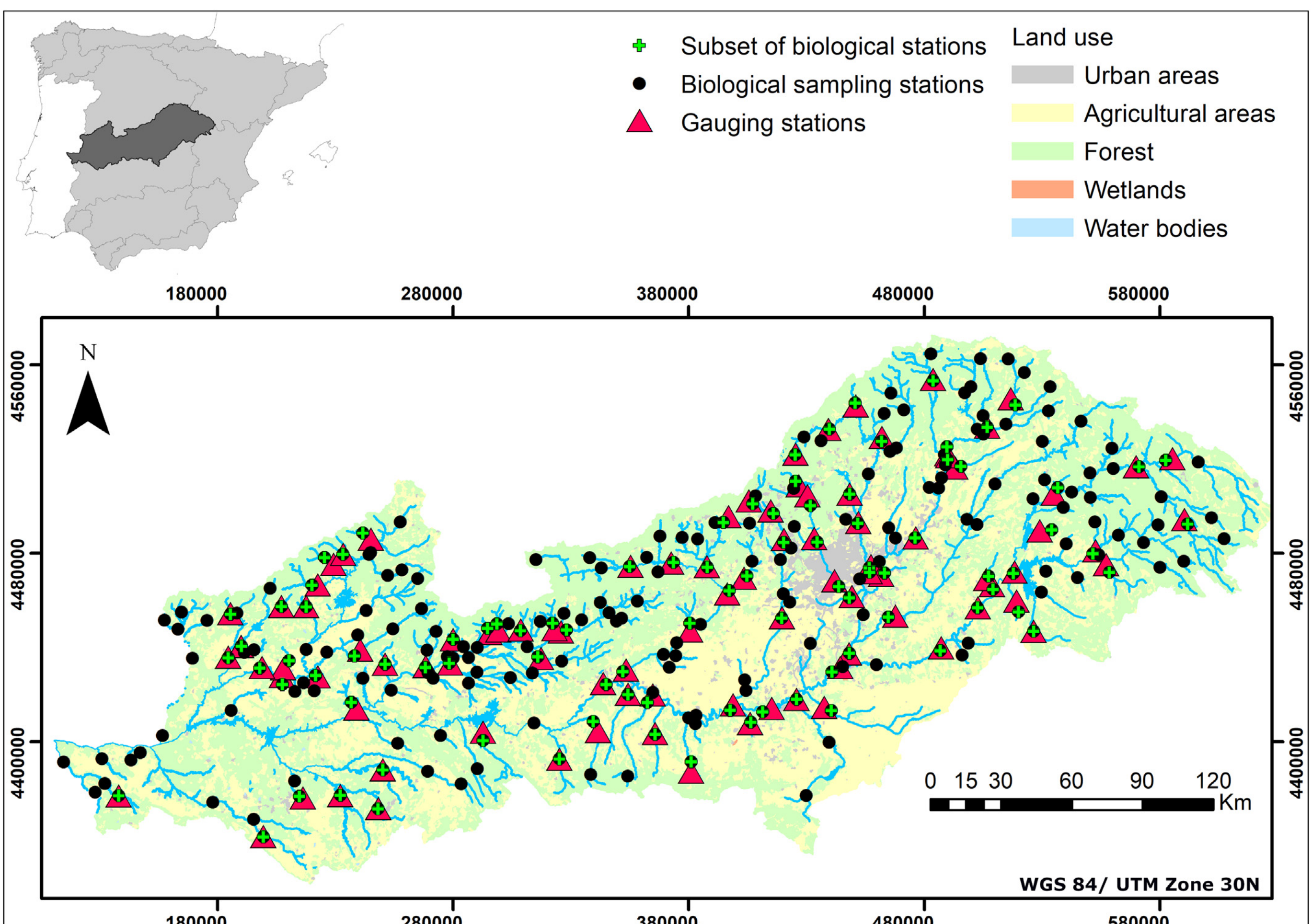

Fig. 1. Map of the Spanish part of the Tagus river basin with the sampling points used in this study. The inset shows the location of the study area in the Iberian Peninsula.

metropolitan area of Madrid, where the density reaches a value of 810 hab/km^2. The intense human activity leads to a high number of pressures acting on the basin including hydromorphological alterations, water abstraction, and point and diffuse pollution, especially related to urban discharge and agriculture. The volume of groundwater directly exploited is lower than the national average. Aquifers are mostly seen as a strategic water source during severe droughts or to meet local water needs. Moreover, they are key in the maintenance of the base flow in rivers. According to the Tagus river basin Management Plan 2015–2021 (CHT, 2015a), the ecological status of the surface water bodies is good or very good in about 58% of water bodies, less than good in 41% and unknown in 1%. The Plan identifies the high number of dams in the basin, the discharge of treated wastewater of Madrid, a large transfer of water from the Tagus River headwaters and the water abstraction to meet the demand in the Madrid region, as the main pressures that hamper the achievement of a good ecological status. Moreover, recent studies reveal that climate change will particularly affect the Tagus basin in the future (CEDEX, 2017), with an expected reduction in water resources availability.

2.2. Data availability

This study aims at quantifying the ecosystem response to the stressors acting in the Spanish part of the Tagus river basin. Data characterizing the biological and stressor variables were retrieved from several sources. We used the data provided by the CEMAS network (acronym in Spanish for surface water quality monitoring network), a monitoring network set up in 2006 to provide biological, physico-chemical and hydromorphological data for each water body. In the study area, this network has 258 quality sampling points (dots in Fig. 1), one for each water body, with data available for 11 years during the period 2006–2018 (data for 2011 and 2012 were unavailable). The final number of stations considered, after removing the instances with missing values, was 236 for both indices. Hydrological data were obtained for the gauging stations shown with triangles in Fig. 1. In order to relate biological and hydrological data, sampling stations of the CEMAS network located at a maximum distance of 5 km to a gauging station (crosses in Fig. 1) were selected (70 in total). Finally, data from 2012 Corine Land Cover survey (European Environmental Agency, 2016) were used to compute land cover statistics.

2.2.1. Biological data

The dataset included the values of the national freshwater biological quality indices computed for three BQEs: macroinvertebrates, diatoms and macrophytes. For the macroinvertebrates, this is the IBMWP (Iberian Biomonitoring Working Party), which is based on the sensitivity of the aquatic invertebrate community to organic pollution (Alba-Tercedor et al., 2002). The index for diatoms is IPS (Indice de Polluosensibilité Spécifique) (Coste, 1982), based on the weighted averaging equation by Zelinka and Marvan (1961) that reveals the presence of eutrophication, organic matter, acidification and salinity (Almeida et al., 2014). The IBMR (Macrophyte Biological Index for Rivers) is employed for macrophytes, which is an indicator of the trophic status and organic pollution (Haury et al., 2006). The biological sampling campaigns are usually carried out in spring (when the biological communities reach their maximum density and diversity and thus considered the best monitoring period) in the dots shown in Fig. 1 and following the standard protocol approved by the Spanish ministry in charge of environmental affairs. The values of IBMWP and IPS biological indices were used as response variables in the model. Eventually, the IBMR index was excluded due to the insufficient number of available observations.

2.2.2. Stressor variables

In order to have a complete picture of all the pressures acting on the system, we considered all the stressor variables listed in Table 1, which

Table 1
List of stressors used as explanatory variables in the model.

Stressor group	Metric code	Metric description
Pysicho-chemistry[a]	Cond.	Annual mean conductivity (μS/cm)
	pH	Annual mean pH (−)
	O_2	Annual mean concentration of dissolved oxygen (mg/l)
	NH_4	Annual mean concentration of Ammonium (mg NH_4/l)
	PO_4	Annual mean concentration of Phosphate (mg PO_4/l)
	NO_3	Annual mean concentration of Nitrate (mg NO_3/l)
Land use[b]	%_agr	% area of agriculture in the upstream basin
	%_for	% area of forest areas in the upstream basin
	%_urb	% area of urban areas in the upstream basin
	urb_disch#	Number of urban wastewater discharges in the upstream basin (number/km^2)
Hydromorphology Dam impact indicators	dist_dam_ds	Distance to the nearest downstream dam/weir (km)
	dist_dam_us	Distance to the nearest upstream dam/weir (km)
	ds_dam#	Downstream dam/weir density (number/km)
	us_dam#	Upstream dam/weir density (number/km)
	catch_dam#	Dam/weir density in the upstream basin (number/km^2)
Effect of tributaries	us_trib#	Upstream tributaries density (number/km)
	ds_trib#	Downstream tributaries density (number/km)
Physical-habitat structure[a]	QBR	Riparian Forest Quality Index (−)
Hydrology[c]	Q_mean	Annual mean flow divided by upstream basin area (m/s)
	Q_min	Annual minimum flow divided by upstream basin area (m/s)
	Q_max	Annual maximum flow divided by upstream basin area (m/s)
	base_flow	Base Flow: the minimum of a 7-day moving average flow for each year divided by the annual mean flow for that year (−)
	zero#	Number of days with zero flow (−)
	low#	Number of low pulses-periods during which the flow falls below 25th percentile of the entire flow record (−)
	high#	Number of high pulses-periods during which the flow exceeds the 75th percentile of the entire flow record (−)
	L_low	Duration of low pulses (number of days)
	L_high	Duration of high pulses (number of days)
	rise	Rise rates: mean of all positive differences between consecutive daily values (m/s)
	fall	Fall rates (m/s): mean of all negative differences between consecutive daily values (m/s)
	rev#	Number of reversals (−): number of days in each year when the change in flow from one day to the next changes direction
Environmental descriptors	Altitude	Altitude (m asl)
	us_catch_area	Upstream catchment area (km^2)
	WFD_typ	Environmental typology of the stations (−)
Temporal-spatial covariates	Date	Biological sampling date (days)
	X_coord/Y_coord	Coordinates of sampling station (UTM)

[a] From Red CEMAS (data recollection four times a year).
[b] From 2012 Corine Land Cover.
[c] From gauging stations.

account for the effects of urban wastewater discharges, land use cover, hydromorphological alterations and river flow regime.

Physico-chemical parameters were retrieved from the Spanish monitoring programme that samples river quality four times a year (to capture the seasonal variation) in the CEMAS network. The following physico-chemical variables were used in the study: conductivity (μS/cm), ammonium (mg NH_4/l), phosphate (mg PO_4/l), nitrate (mg NO_3/l), dissolved oxygen (mg/l) and pH. Due to the different sampling frequency of the biological indices (once a year) and the physico-chemical parameters (four times a year), a temporal aggregation was needed. As in Meißner et al. (2019), for each parameter all the physico-chemical measures collected in the 12 month period prior to the biological sampling date of IBMWP and IPS were averaged.

The 2012 Corine Land Cover survey data was used to compute the land uses in the upstream catchment area of each sampling station. The Corine Land Use classes were aggregated into three categories: agriculture, urban and forested areas. Land-use is a proxy for different stressors rather than a stressor itself (Segurado et al., 2018). However, its high predictive value, demonstrated in several studies (e.g. Theodoropoulos et al., 2015), justifies its use as an input variable for the model.

The hydromorphological stressors were characterized through the Riparian Forest Quality Index (QBR), which evaluates the riparian habitat quality of streams in terms of total vegetation cover and tree composition (Munné et al., 2003) and through several indices of hydromorphological alteration. Following the approach proposed by Wang et al. (2011) and Van Looy et al. (2014), we used the following parameters for each monitoring point: the density of the upstream and downstream dams (and weirs) and the distance to the nearest dam (and weir). The effect of the tributaries in terms of sediment load supply was included by computing the upstream and downstream tributaries density, consistently with the metrics recommended in Cumming (2004).

As suggested in Feld et al. (2016), three environmental descriptors were also factored in to account for natural variability in the basin: altitude (m asl), upstream catchment area (km^2) and the typology of the surface water body. The latter variable refers to the classification of ecotypes requested in the Annex II of the WFD and carried out for Spain in CEDEX (2004) (Table S1, Supplementary material).

In order to avoid temporal pseudo-replication, we also added the biological sampling date expressed as Julian date and the coordinates of the sampling stations as temporal and spatial covariates, respectively (see Feld et al., 2016). Additionally, we cleaned the dataset to ensure that each station was sampled only once a year (Kakouei et al., 2018; Meißner et al., 2019).

In addition to the above variables, hydrological variables were computed for the gauging stations. This choice was supported by the evidence that hydrology significantly affects the response of biological communities (Meißner et al., 2019; Palmer and Ruhi, 2019; Poff et al., 2006). The indicators of hydrological alteration (IHA) developed by the Nature Conservancy (2009) were used as a reference. Daily discharge data for each gauging stations were acquired from the Tagus River Basin Authority and the metrics were computed by averaging the data for the year prior to the biological sampling date. Among the 33 available IHA parameters, which characterize the flow regime in five hydrological dimensions (magnitude, frequency, duration, rate of change and timing), we selected those shown in Table 1. Some of the metrics (Q_mean, Q_min, Q_max) were divided by the catchment area, in order to normalize them and to allow for the comparison across different sampling points.

2.3. Empirical modelling: predicting biological response to stressors

Two machine learning algorithms were applied: Random Forest (RF) (Breiman, 2001) and Gradient Boosted Regression Trees (GBRT) (Friedman, 2001). They are both ensemble methods that use binary decision trees as base learner. They use two different training strategies: randomization in the case of RF (i.e. training a set of randomized decision trees, where each model is trained on a random bootstrap sample of the data) and optimization in case of GBRT (i.e. training a set of individual models in series, learning by gradient descent the residuals not learnt by the previous submodels).

These algorithms have proven to perform rather well in different fields of application (Zhang et al., 2017). They are suitable to address cases where a large number of independent variables have to be considered (Feld et al., 2016). Moreover, they are able to identify non-linear relationships. Note that, as a preliminary analysis, we applied linear regression to the data and non-optimal results were obtained. Finally, they allow for the quantification of the importance of variables (Breiman, 2001). All these elements are present in this study and motivated the selection of RF and GBRT.

The variables of the present analysis are not affected by strong collinearity. Thus, all the variables were included in the analysis. The Variance Inflation Factor (VIF) was used to compute the correlation among variables. The value of VIF was found to be below 8 for all possible variable relations, a threshold usually set to identify variance-inflated variables (Feld et al., 2016).

The analysis included the evaluation of the model performance, followed by the assessment of the stressors hierarchy. In order to obtain accurate estimates of the model performance, a k-fold cross-validation (with $k = 10$) was applied. The original dataset was divided into k disjoint subsets of equal size; then each of the k subsets was retained once to test the models trained on the remaining k-1 subsets. Finally, the generalization errors obtained from the k left-out sets were averaged to produce the final performance estimation. This method yields more stable results than using a single random train/test partition and provides an independent validation for each of the available observations. To conduct RF and GBRT analysis, the functions *RandomForestRegressor* and *GradientBoostingRegressor* of the Python package *scikit-learn* (Pedregosa et al., 2011) were used. Regarding the RF model hyperparameters, the number of trees in the forest was set to 500 - a number large enough for the ensemble to converge - while the number of variables to consider when looking for the best split was set to the logarithm of the total number of independent variables (Breiman, 2001). These parameters were used for all the experiments. In contrast, in GBRT, the hyperparameters need to be optimized. In order to carry out this process, an in-train nested k-fold cross-validation-grid search was performed to tune the learning rate (grid values: 0.05, 0.1, 0.5) and the maximum depth of the individual regression tree estimators (grid values: 2, 3, 7, 11), testing a range of values around the default values of the algorithm. The combination of hyper-parameters that provided the lowest mean squared error in the nested cross-validation was then used to train the GBRT model on the whole training set.

The algorithms were trained to predict both biological indices, IBMWP and IPS. The quality of each model was assessed computing the coefficient of determination (R^2), the root mean square error (RMSE) and the mean absolute error (MAE). Once the best performing model between RF and GBRT was identified, the stressors were ranked by applying the permutation importance method on the best model. The importance of each variable was determined by computing the increment of the model's prediction error after randomly shuffling the given variable (Breiman, 2001). A greater percentage of increase means a greater impact of the variable on the predictions. Finally, the marginal effect that one variable has on the predicted outcome of the model was visualized by a partial dependence plot (Friedman, 2001). The variable importance and the partial dependence were obtained for each of the k iterations of the cross-validation procedure and the final results were the average over the 10 folds.

We assessed the performance of the models in predicting the status class of the biological indices in order to understand their potential to classify the ecological status of a water body. For this purpose, the IBMWP and IPS values given by the regression models were classified

Table 2
Description of scenarios tested to predict the status of IBMWP and IPS indices.

Scenarios	Nutrients	NO3 (mg/l)	NH4 (mg/l)	PO4 (mg/l)	QBR
0	Annual mean 2018				2018 value
SPAIN_THR	Maximum nutrient concentration threshold	25	0.6/1[a]	0.4/0.5[a]	2018 value
SPAIN_THR_QBR	set by the Spanish legislation				Ref. value
50th_EU	50th percentile of the nutrient values	12	0.39	0.3	2018 value
50th_EU_QBR	established by EU legislations				Ref value
25th_EU	25th percentile of the nutrient values	7	0.2	0.2	2018 value
25th_EU_QBR	established by EU legislations				Ref. value
75th_GOOD	75th percentile of nutrient concentrations in the water	6	0.1	0.27	2018 value
75th_GOOD_QBR	bodies classified as good in the Tagus basin				Ref. value

[a] Depending on the water body type (see MAPAMA, 2015).

into "less than good" and "good/very good" by applying the thresholds of the biological indices for each status class as are defined in MAPAMA (2015) (Table S1, Supplementary material).

Due to the limited coverage of the hydrological data (instream flows), the analysis was carried out for two different datasets: the whole set of CEMAS stations without considering the hydrological variables and a subset of CEMAS stations close to the gauging stations where the relevant hydrological data were available.

2.4. Definition of scenarios

The best fitting algorithm among RF and GBRT (i.e. the one with the highest R^2 in the previous phase) was used to predict the biological indices under different scenarios. A simplified model was built selecting the nutrients and the variables with the highest explanatory power according to the feature importance analysis. Among them, the variables urban wastewater discharges in the upstream catchment area and the conductivity are correlated with nutrients. Since it was not possible to precisely quantify their correlation with the nutrient concentrations set in the scenarios, those variables were excluded from the simplified model.

For each station we built a model using all the training data except those of the station itself. The resulting models were used to predict the expected biological indices in each water body under nine scenarios combining different nutrient concentrations (ammonium, nitrate and phosphate) and QBR values (Table 2). For each possible scenario the oxygen concentration was varied between the minimum measured value and the most favourable value of 11 mg/l. This value was obtained by computing the 75th percentile of oxygen distribution in all the water bodies classified as good in the study area.

To build the scenarios, for the hydromorphological index QBR we considered two possible values: the value measured in 2018 and the value representing the reference condition for each water body type defined for Spain in MAPAMA (2015) (see Table S1 Supplementary material). As for the nutrient values, we defined four different options. The first one corresponds to the maximum nutrient concentration thresholds (SPAIN_THR) set by the Spanish legislation to ensure the good ecological status (MAPAMA, 2015). The second (50th_EU) and the third (25th_EU) thresholds correspond to the 50th and the 25th percentile of the nutrient values established by the legislation of other EU countries, respectively. The data for phosphate and nitrate in the different EU Member States were obtained from Phillips and Pitt (2016) while Claussen et al. (2012) report the threshold values for ammonium. Finally, the fourth values for nutrient concentrations (75th_GOOD) were obtained by applying a method frequently adopted by Member States to set quality standards (Phillips and Pitt, 2016). This considers the 75th percentile of the distribution of nutrient concentrations in all the water bodies classified as good. The scenario with the values measured in 2018 for nutrients and QBR index was also considered as a baseline, obtaining the nine scenarios listed in Table 2.

The scenarios were firstly used to focus on a small number of sampling points, in order to investigate the sensitivity of the status of the biological indices to the explanatory variables considered. We selected three sampling stations located in the middle Tagus basin (Fig. S1, Supplementary material), which is the region with the highest number of water bodies in less than good status. These are TA13242 (Manzanares river), TA12110 (Jarama river) and TA12151 (left tributary of Tagus river). For the water bodies associated with the stations TA13242 and TA12110, the Spanish legislation establishes less stringent environmental objectives, setting higher nutrient thresholds. Therefore, in this case we considered two additional scenarios: LESS and LESS_QBR. In these two scenarios, the less stringent nutrient thresholds defined in the Spanish legislation are associated to the QBR index measured in 2018 and its reference value, respectively.

We then tested the scenarios listed in Table 2 in all the stations where the IBMWP and IPS indices are currently classified as less than good. The aim of this step was to understand how the classification of the status of the water bodies would vary in the entire basin in the different scenarios considered in this study.

3. Results

3.1. Quality of the model

The evaluation of the quality of the model was based on the values of the prediction statistics for the testing dataset. In this first analysis, we used the data from the 236 CEMAS stations without considering the hydrological stressors. The RF and GBRT models were used to predict the annual values of the IBMWP and IPS indices in each station of the study area. The comparison of the statistics R^2, RMSE and MAE shows that RF performs slightly better than GBRT in modelling both biological indices (see Table 3) and thus it was selected to compute the subsequent analysis. The comparison between observed and modelled values for RF model is shown in Fig. S2.

The confusion matrix (see Table S2, Supplementary material) reveals that RF model performs well in predicting the two classes of biological status for both IBMWP and IPS indices, with a percentage of correct identification that ranges between 74% and 90%.

3.2. Variable importance

The feature importance analysis in the IBMWP predictive model reveals that the categories of land cover in the upstream catchment area and the concentration of ammonium are ranked as the main variables

Table 3
Prediction statistics for IBMWP and IPS indices.

	IBMWP			IPS		
	R^2	MAE	RMSE	R^2	MAE	RMSE
RF	0.76	21.32	28.13	0.73	1.54	2.03
BRT	0.75	21.39	28.36	0.72	1.55	2.05

at play (Fig. 2). The elevation turns out to be the most relevant environmental variable. The hydromorphological parameters have a lower relevance in the model, except for the QBR. In the IPS predictive model, the percentage of urban area in the upstream catchment area and the concentration of ammonium are among the three top variables, together with the conductivity parameter. The number of dams in the upstream basin and the QBR index appear to be the most important hydromorphological variables, while the other variables of this category maintain a lower explanatory power. The environmental type of the water body is an important predictor for both indices. Nitrate and dissolved oxygen appear to be relevant in the IBMWP model, while the number of urban wastewater discharges in the upstream drainage area and the phosphate concentration notably affect the IPS index.

3.3. Partial dependence plot

According to the partial dependence plots shown in Fig. 3, the following variables present a negative effect on the IBMWP index: ammonium, conductivity, nitrate, phosphate, size of the upstream area, urban and agriculture land coverage. On the contrary, QBR, oxygen, elevation, and forest land coverage positively affect the IBMWP index.

In the case of ammonium, nitrate, conductivity, agriculture and urban land cover the impact on the response variable appears stronger for lower values of the variable. The IBMWP index first shows a steep decrease and then, with the progressive increase of the variables, remains nearly constant. On the contrary, higher values of QBR, percentage of forested area and elevation have a more marked effect. The IBMWP index does not strongly respond to the remaining variables, as confirmed also by the low score attributed to them in the variable importance analysis.

The sign of the relationships between the IPS index and the explanatory variables remains the same as in the model of the IPBWP index. Again, it is possible to observe a stronger relationship for lower values of conductivity and percentage of urban land cover.

3.4. The role of the hydrological explanatory variables

An additional analysis was undertaken with a subset of stations where also the hydrological explanatory variables were available. This is to evaluate the impact of hydrological variables on the model.

RF and GBRT perform similarly (see Table S3, Supplementary material). The analysis of the variable importance reveals that the hydrological variables do not have a high explanatory power (Fig. S3, Supplementary material). In the IBMWP model, the first hydrological variables in the ranking are the specific maximum and mean discharge (ranked 21st and 22st, respectively), while in the IPS model the number of reversals is ranked 17th. Moreover, the quality of IBMWP and IPS model remains the same when run on the same subset without the hydrological variables, thus confirming to be weakly dependent on the hydrological metrics. Furthermore, a model built only on the hydrological and environmental variables can explain only the 33% of the variance of the modelled variables.

3.5. Predictions of IBMWP and IPS indices for different scenarios

Due to its higher accuracy and given the low impact of the hydrological variables, we used the RF algorithm trained on the entire dataset to predict the biological indices under different scenarios. The variables chosen to build the simplified IBMWP and IPS model are listed in Table 4, together with the model accuracy (R^2) obtained when trained only on those variables. For the stations TA13242, TA12110 and TA12151, we analysed the trend of the biological response (IBMWP index) as function of nutrient concentrations, QBR and oxygen in the three sampling points (Fig. 4a–c). Each box plot in the figures shows the variation of the IBMWP value according to the oxygen concentration, which varies between the minimum measured value and the most favourable value of 11 mg/l.

In all the sampling stations, the values of the IBMWP index improve when imposing lower nutrient values. The nutrient concentrations associated to the less stringent objective lead to a very low IBMWP value: both stations TA13242 and TA12110 are classified as poor in

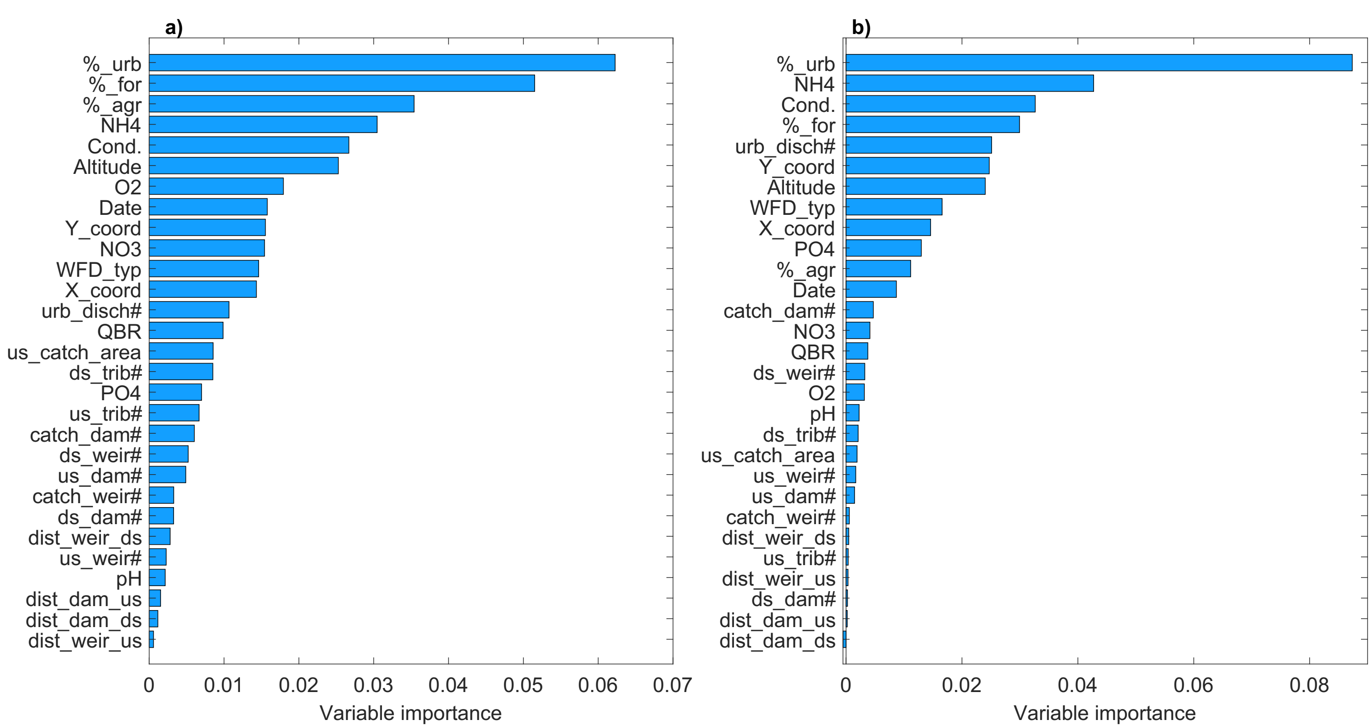

Fig. 2. Ranking of variable importance in the IBMWP (a) and IPS (b) predictive models. For the metric codes of the variables see Table 1.

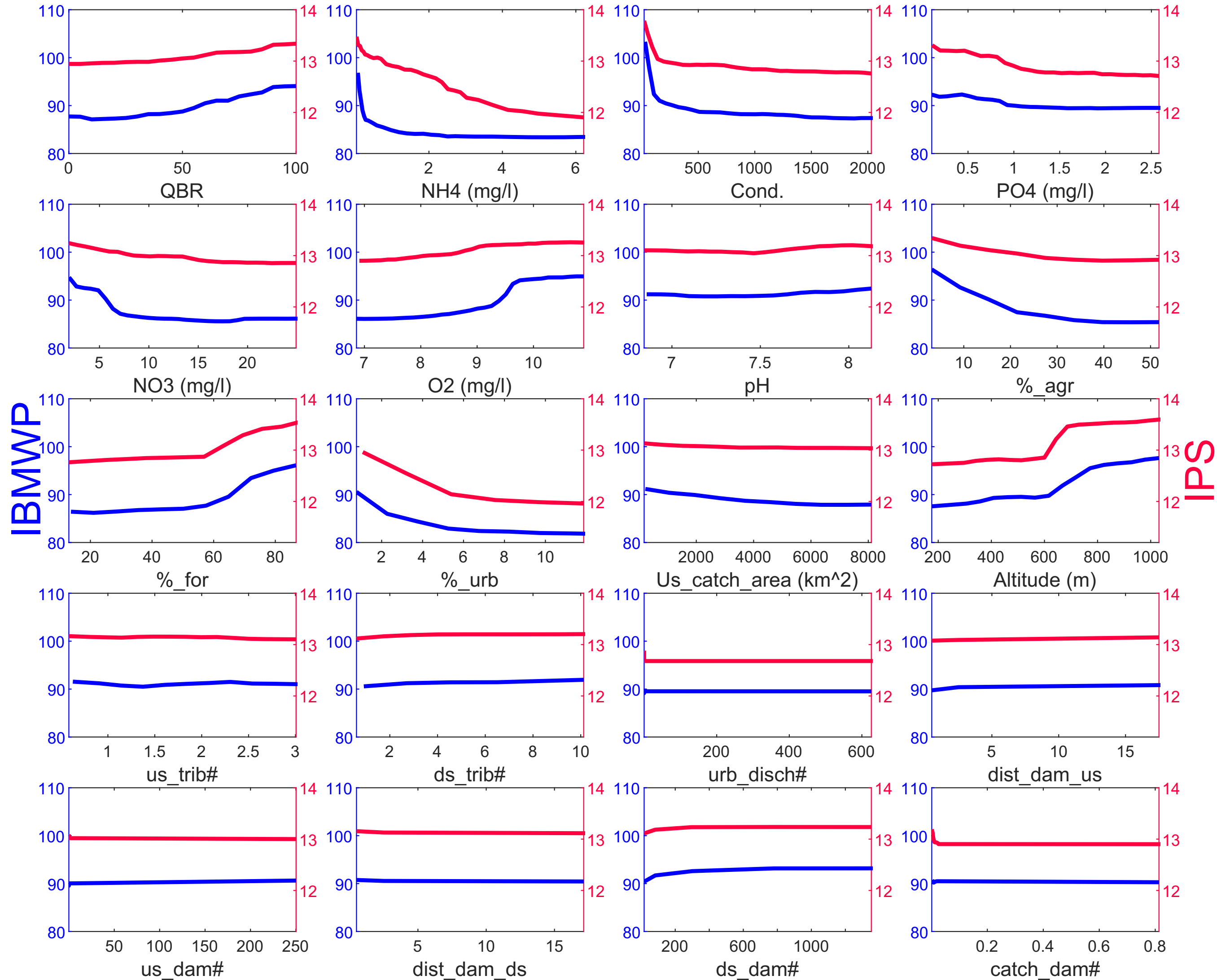

Fig. 3. Partial dependence plot of the explanatory variables in the IBMWP (blue line) and IPS (red line) predictive models. For the metric codes of the variables see Table 1. The results for the variables catch_weir#, dist_weir_us, dist_weir_ds, us_weir# and ds_weir# are not reported in the figure because not significant.

the scenario LESS. In all the cases, a significant range of variation of IBMWP results by varying the oxygen value and the QBR index: higher values of oxygen concentration and QBR index lead to a higher IBMWP index. The most favourable values of IBMWP are reached in the scenario 75th_GOOD_QBR, especially when a high oxygen value is set: stations TA13242 and TA12151 reach the good status; station TA12110 is still classified as moderate, but the improvement with the respect to the scenario 0 is significant.

After running the model only for those three sampling stations, we tested the scenarios listed in Table 2 in all the stations where the IBMWP and IPS indices are currently classified as less than good (see Fig. 5a–b).

We considered the values measured in 2018 (scenario 0 in Table 2) as a baseline. For the IBMWP index, 46% of the total number of stations are classified as less than good (108 out of a total of 236 stations), with 7 stations in bad status, 36 in poor status and 65 in moderate status. The IPS index is less than good in 39% of the stations, with 25 stations in bad status and 68 in moderate status.

For the IBMWP index, the number of stations with good status increases in all scenarios as the nutrient threshold becomes more restrictive. For instance, when comparing scenarios 0 and 75th_GOOD (see Table 2 for the values of nutrient concentrations), the total number of stations in good status increases by up to 48% (from 128/236 in scenario 0 to 189/236 in 75th_GOOD). This trend is even more evident when a QBR index higher than the one measured in 2018 is imposed. In scenario 75th_GOOD_QBR, in the case of a favourable value of oxygen (lower whisker in Fig. 5a), the number of stations with a less than good status is reduced to about 1/3 with respect to the baseline and no station is classified as bad or poor (see Fig. 6). The trend identified for the IBMWP index is confirmed also in the case of the IPS index, even if is less pronounced: the number of station with a less than good status in

Table 4
Explanatory variables selected for the simplified IBMWP and IPS models and corresponding precision expressed as R^2.

Biological indices	Explanatory variables	R^2
IBMWP	%_agr, %_for, %_urb, NH_4, NO_3, PO_4, O_2, QBR, Altitude,WFD_typ, Us_catch_area, Date, X_coord, Y_coord	0.75
IPS	%_agr, %_for, %_urb, NH_4, NO_3, PO_4, QBR, Altitude, WFD_typ, catch_dam#, Date, X_coord, Y_coord	0.73

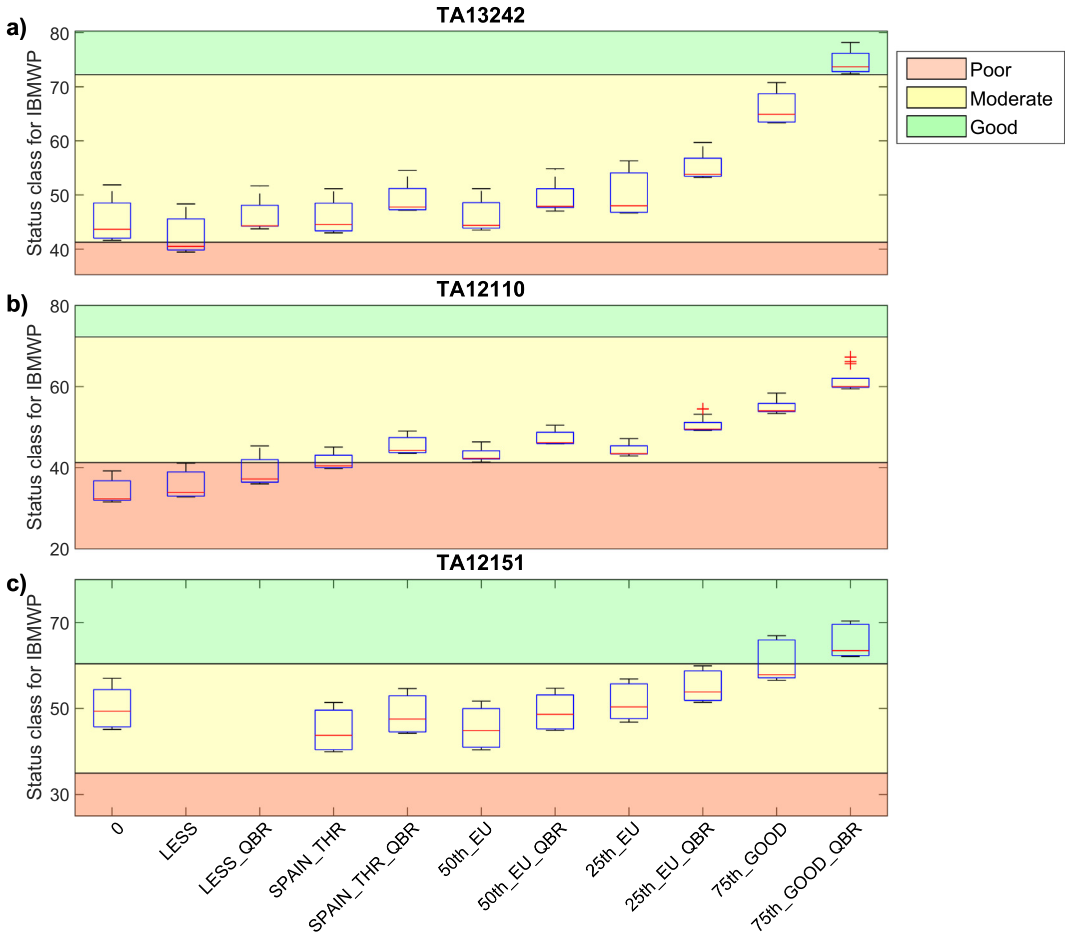

Fig. 4. Classification of the status of IBMWP in the stations TA13242 (a), TA12110 (b) and TA12151 (c) for the different scenarios of Table 2. In the case of TA13242 (a) and TA12110 (b), stations subjected to less stringent environmental objectives, two additional scenarios (LESS and LESS_QBR) are considered. Nutrient concentrations (in mg/l) in the scenario 0 are: $NH_4 = 0.19$, $PO_4 = 0.9$, $NO_3 = 18$ (a); $NH_4 = 7$, $PO_4 = 0.9$, $NO_3 = 13$ (b); $NH_4 = 0.2$, $PO_4 = 0.9$, $NO_3 = 10$ (c). Nutrient concentrations (in mg/l) in the scenario LESS and LESS_QBR are: $NH_4 = 10$, $PO_4 = 0.5$, $NO_3 = 25$ (a); $NH_4 = 8$, $PO_4 = 0.5$, $NO_3 = 25$ (b).

general decreases progressively by reducing the nutrient concentrations and by increasing the QBR index values. The status of the water bodies improves in about 28% of the total sampling points, but in 53 stations it remains less than good even in the most favourable scenario (75th_GOOD_QBR).

4. Discussion

4.1. Modelling results

RF and GBRT successfully modelled the values of biological indices for macroinvertebrates (IBMWP) and diatoms (IPS) using data from different categories of explanatory variables. It was not possible to include the biological index for macrophytes (IBMR) in the analysis, due to the insufficient number of available observations. Each model was trained on two different sets of explanatory variables: the complete dataset without hydrological stressors and a subset of stations that also includes the hydrological independent variables. In most cases, RF is found to perform slightly better than GBRT. For both indices and for both sets of data, the modelling quality can be considered satisfactory (Moriasi et al., 2007), especially when the model was fit on the entire dataset. The modelling performance is comparable with other studies predicting different kinds of bioindicators with the use of Decision Tree algorithms (Holguin-Gonzalez et al., 2013; Lopatin et al., 2016; Álvarez-Cabria et al., 2017; Grizzetti et al., 2017). The modelling performance results particularly good also compared to the accuracy of other empirical models used to predict biological quality indices (Gebler et al., 2018; Liu et al., 2020).

The analysis of the hierarchy of stressors reveals that the categories of land cover in the upstream catchment area and the nutrient concentrations (especially ammonium) are the most relevant variables in IBMWP and IPS models. The high relevance of land use variables is further evidence of nutrient importance as explained in Segurado et al. (2018): agricultural land cover can be considered a proxy for diffuse pollution in form of nutrients; urban areas and the number of urban wastewater discharges are representative of point pollution; and forested lands are a proxy for processes that contribute to filter water pollutants. The predominance of land use variables and nutrient concentrations variables have been found also in other case studies (Herrero et al., 2018; Segurado et al., 2018). Similar findings were also confirmed at a European scale by Grizzetti et al. (2017).

Geo-environmental variables, such as elevation and the typology of the water body, also notably affect the values of the indices. Among the hydromorphological variables, QBR turns out to be the most relevant variable in both models, together with the number of dams in the upstream catchment area in case of the IPS model. The hydrological variables do not stand out as the most important ones. In contrast to our findings, several studies in literature underline the importance of the IHA metrics in explaining the response of the biological communities (e.g. Leigh and Datry, 2017; Meißner et al., 2019) and the link between ecosystem and alteration of the hydrological regime is widely accepted (Palmer and Ruhi, 2019). Thus, it would be interesting to further explore the role of the hydrological variables on the status of water bodies in our

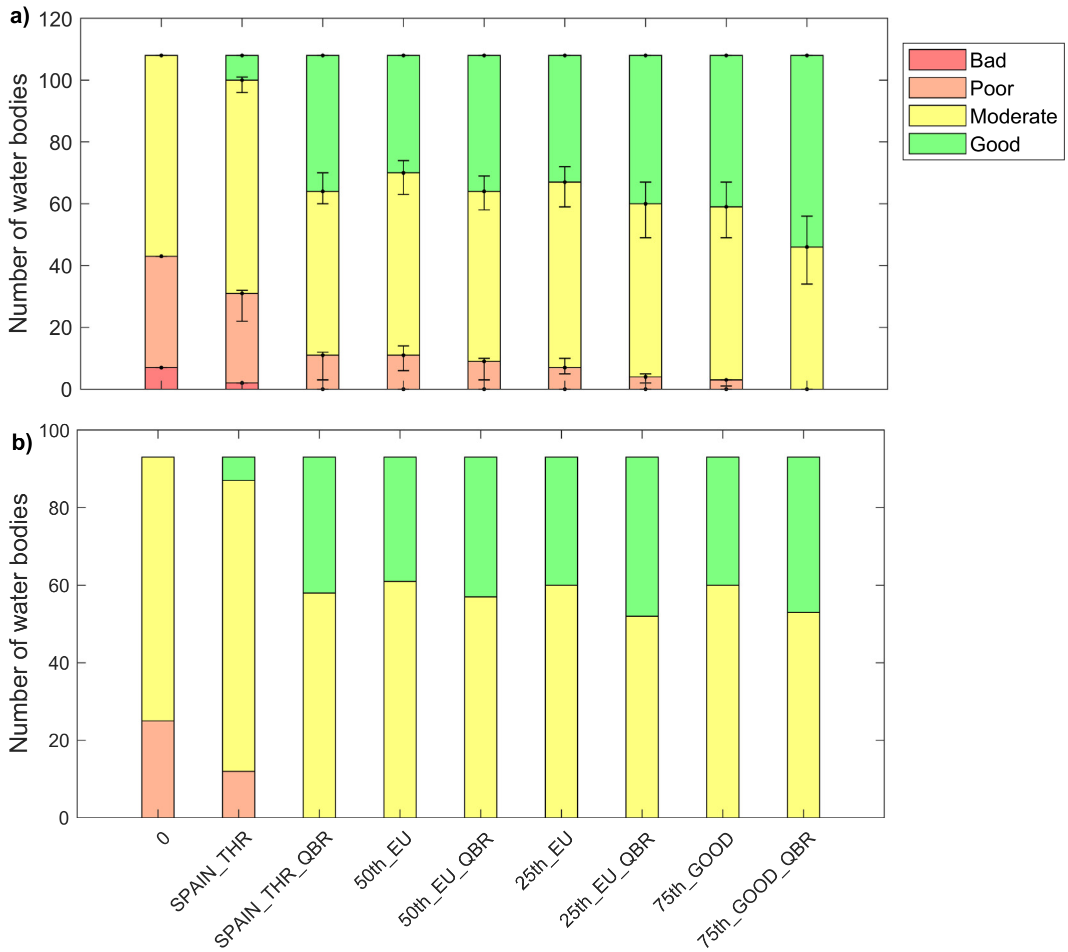

Fig. 5. Number of water bodies in the different categories of status of the IBMWP (a) and IPS (b) index in the different scenarios of Table 2. The whiskers in panel a show the range of the results by varying the oxygen concentration between the minimum and the most favourable value.

case study. Due to data availability, we had to limit the analysis of the impact of the hydrological variables to a reduced subset of stations and to the BQEs measured. Performing the analysis on a larger subset and including fish among the response variables as a taxonomic group particularly sensible to hydrological alteration (Merciai et al., 2017) might yield different results. We chose to compute the IHA metrics in the 12 months antecedent to the biological sampling date, a period considered relevant to describe the effect of recent, often extreme, hydrological events on biological communities (Leigh and Datry, 2017). Nevertheless, other authors found interesting results computing hydrological metrics over a longer time period (e.g. Lynch et al., 2018; Steel et al., 2018). Thus, in the future it could be interesting to compute IHA metrics over different time periods in our case study to further characterize the relations between hydrological and biological variables. The results of the hydrological analysis may also be influenced by the distance between the biological sampling stations and dams. Mellado-Díaz et al. (2019) showed that the IBMWP index generally decreases below dams, thus suggesting that a higher number of biological samples could better detect the longitudinal trends in the hydrological impact along the river.

To fully evaluate the alteration of the hydrological regime, the groundwater contribution should also be taken into account. Groundwater ensures base flows and habitat connectivity (Falke et al., 2011), and thus its exploitation can affect the persistence of aquatic ecosystems (Falke et al., 2011; Perkin et al., 2017; Bui et al., 2020). In this perspective, an integrated management of surface and groundwater resources is crucial to address ecosystem degradation and the conflicts between stakeholders (Kapetas et al., 2019). So far, the effects of groundwater abstraction on stream ecosystems have been poorly investigated, mainly due to the lack of reliable data to quantify groundwater abstractions (Liu et al., 2020). An integrated surface-subsurface hydrological model, as recently developed by Liu et al. (2020), could be an interesting approach to address the issue.

The relationships between stressors and biological indices that emerge from the partial dependence plot mostly confirm expectations. Nutrient concentrations, size of the upstream area, urban and agriculture land coverage negatively affect the IBMWP and IPS indices; on the contrary, QBR, oxygen, elevation and forest land coverage present a positive effect on the status of the ecosystem. In general, the relationships that emerge reflect a non-linear response of the indices with respect to the explanatory variables. A steep variation of IBMWP and IPS values can be observed below (ammonium, nitrate, conductivity, agriculture and urban land cover) or above (QBR, forested area and elevation) a certain threshold.

4.2. Prediction of IBMWP and IPS indices for different scenarios

The RF algorithm fitted on the complete dataset (Section 3.1) was used to predict the IBMWP and the IPS indices under different scenarios of water and river morphology quality. According to our model, the nutrient thresholds set by the Spanish legislation are not strict enough to ensure the good ecological status in all the 236 water bodies considered in this study. It is interesting to note that the nutrient concentration limits in Spain stand among the least restrictive ones in the EU

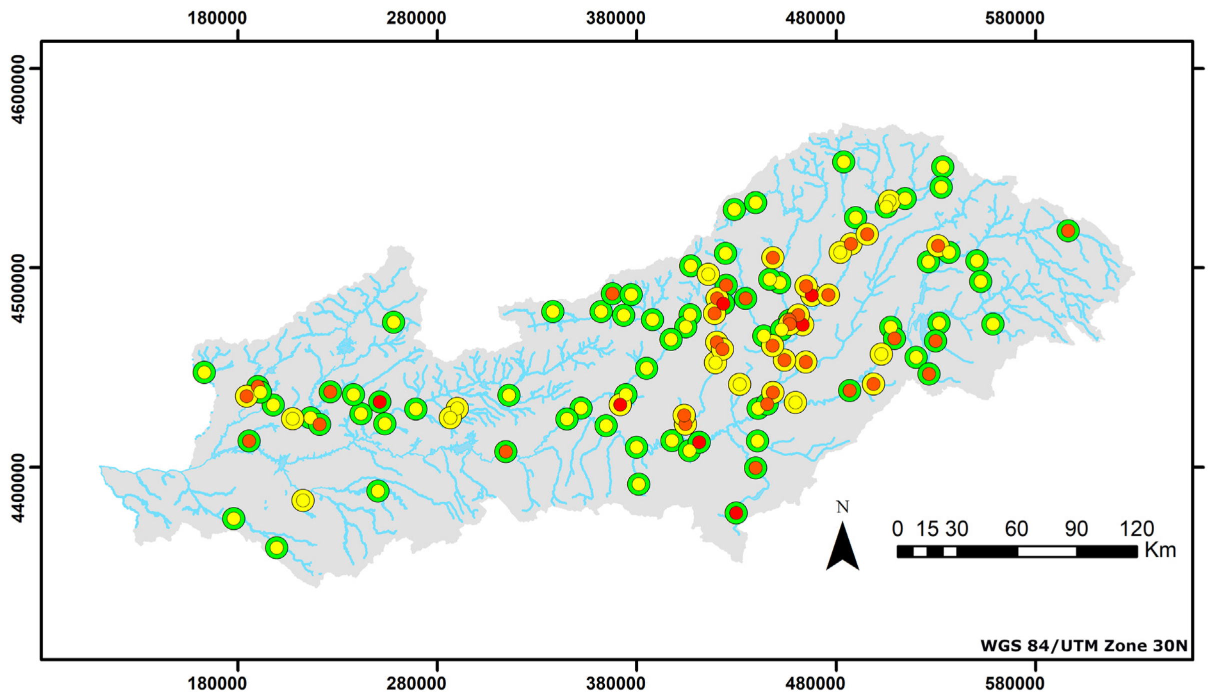

Fig. 6. Classification of the status of the IBMWP index in the scenario 0 (inner dots) and in the scenario 75th_GOOD_QBR in the case of a favourable oxygen concentration (outer dots). The meaning of the colours is: red = bad status, orange = poor status, yellow = moderate status, green = good status.

(Phillips and Pitt, 2016). The Spanish good/moderate threshold value for nitrate nitrogen is a single standard value of 5.65 mg/1 (25 mg/1 as nitrate), which is significantly higher than the EU mean (2.7 mg/l). According to Phillips and Pitt (2016), the value of 5.65 mg/1 is likely to be derived from the guideline value indicated in the now repealed Drinking Water Directive (80/778/EC), although there is no evidence of its link to the ecological status. Also in the case of phosphorous, the Spanish good/moderate boundary value is higher than the EU mean (133 μg/l vs 100 μg/l). The Spanish water authorities based the choice of nutrient concentration thresholds on expert judgment (Phillips and Pitt, 2016), a practice that seems to underestimate the target values, while regression methods were found to be the most recommendable strategy (Dodds and Oakes, 2004; Phillips et al., 2019).

Imposing more restrictive nutrient limits leads to an overall improvement of the water bodies status in the basin. The highest number of stations in good status (up to 189 for IBMWP index and 176 for IPS index out of 236) is achieved by setting the nutrient values limits equal to the 75th percentile of nutrient concentrations in the water bodies classified as good (scenario 75th_GOOD). Thus, the reduction of nutrient concentrations turns out to be effective, but not sufficient to ensure the good status in all the water bodies. In all the scenarios, the positive effect of imposing a high QBR emerges clearly, leading to 85% of water bodies with biological indices in good status in the best case scenario.

These results seem to suggest an interaction between nutrient concentrations and the QBR index. This relation is supported by physical evidence: riparian buffer is proven to retain nitrogen or phosphorus in surface water (Feld et al., 2018), by physically filtering or trapping the nutrients (McKergow et al., 2003). At the same time, Feld et al. (2018) point out that interventions of riparian restoration are not sufficient if they are not coupled with a wider land use management. The two-way Partial Dependence Plots (Friedman, 2001) of the QBR index and the concentration of nutrients further confirm the supposed interaction (Fig. 7): the most favourable values of the biological indices are reached in correspondence of low nutrients concentrations and high values of QBR index.

Therefore, coupling measures of nutrient reduction and improvement of river morphology could be a successful approach. The importance of integrating morphology and water quality confirms the results of other studies. For instance, Gebler et al. (2018) underline the importance of including morphological condition when modelling the ecological status. Theodoropoulos and Iliopoulou-Georgudaki (2010) point out the crucial role of riparian vegetation to the detoxification of rivers, enhancing the water quality status. Grizzetti et al. (2017) show the synergetic effect of maintaining natural floodplains and limiting nitrogen pollution on the ecological status at EU level.

In light of the results, the reduction of nutrients concentration and the improvement of the riparian habitat quality seem crucial to enhance the ecological status. The Programme of Measures of the Tagus river basin Management Plan 2015–2021 (CHT, 2015b) foresees measures to address point pollution (construction of new wastewater treatment plants or strengthening of the existing ones), diffuse contamination (slurry treatment and imposition of rules to regulate the farming practices) and hydromorphological degradation (restauration of riparian vegetation and fluvial connectivity). Our results point to the prioritization of these types of mitigation measures.

Future work could also foresee the use of isotopic analysis to further understand the factors at play in the system. Isotopic analysis has a great potential in understanding the dynamic of the system and the hydrological processes (Barbieri, 2019), as well in identifying the sources and the pathways of contamination (Duvert et al., 2019; Zhang et al., 2018).

5. Conclusions

This paper explores the potential of machine learning techniques to model the biological response to stressors, with the ultimate goal of informing the definition of water policy targets and guiding the design of water management strategies. Random Forest algorithm successfully modelled the IBMWP and IPS indices in the Tagus river basin and allowed the identification of land use categories and nutrient concentrations as the most important features in the system. The model was then used to predict the status of biological elements under different

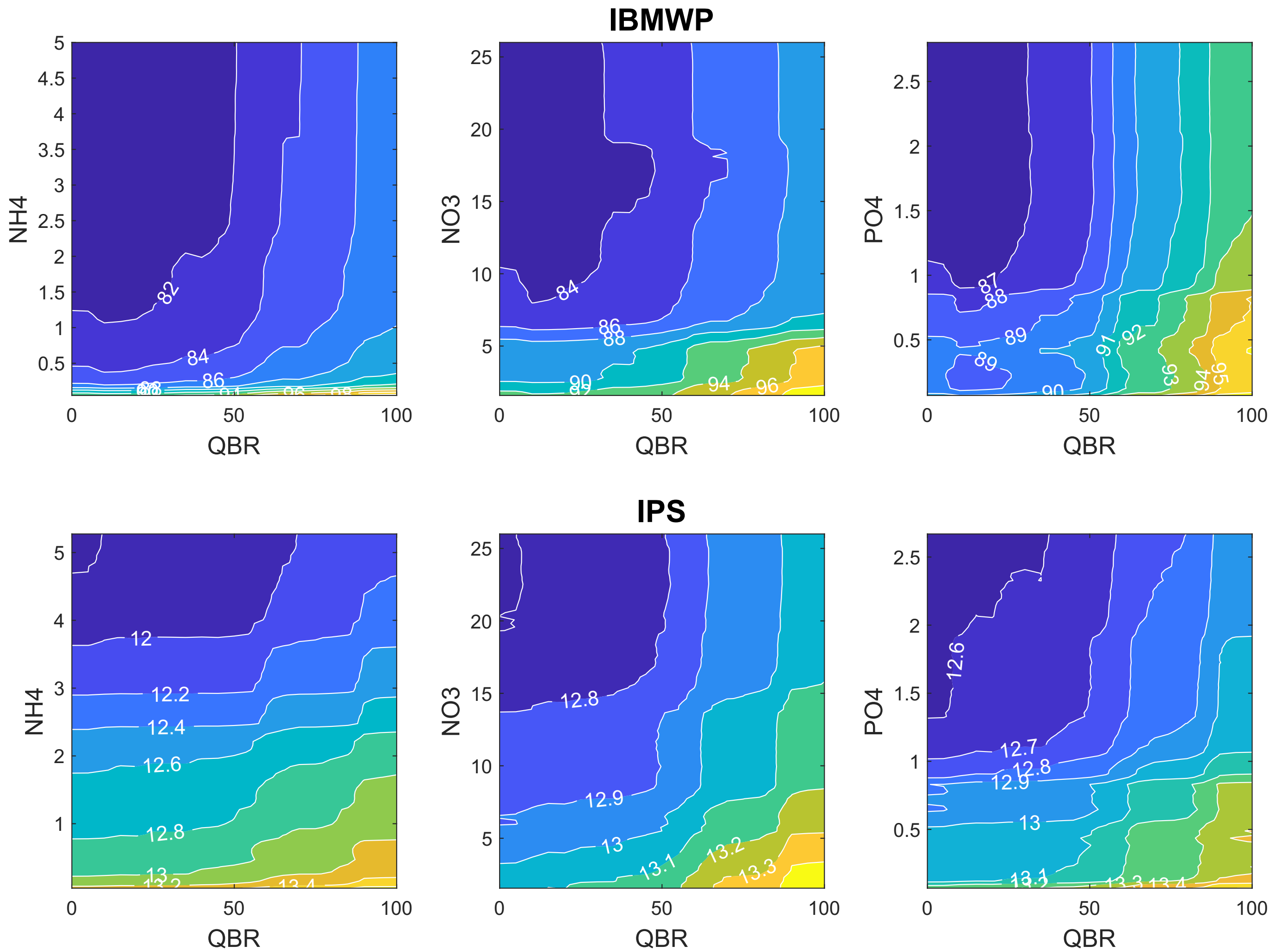

Fig. 7. Two-way partial dependence plot between QBR and nutrient concentrations in the IBMWP and IPS predictive models. For the metric codes of the variables see Table 1.

scenarios of water and river morphology quality. This enabled the evaluation of the effectiveness of current and potential policy measures to improve the quality of freshwater ecosystems, with a special focus on nutrient thresholds.

Setting adequate regulatory targets is essential to achieve the environmental objectives defined by the Water Framework Directive. At present, intercalibrated nutrient thresholds supporting the good ecological status are missing at the European Union level and thresholds for admissible nutrient concentrations vary widely across Member States. This study provides useful insights into the definition of nutrient concentration thresholds adequate to reach a given status of biological indices in a surface water body.

According to our model, the current nutrient thresholds in Spain are insufficient to ensure values of biological indices consistent with the good ecological status in all the water bodies of the Tagus basin. A significant improvement (reaching up to 85% of water bodies with biological indices in good status) could be achieved by coupling more restrictive nutrient thresholds with measures that improve the riparian habitat quality. Thus, this approach appears as a priority mitigation measure to restore the status of freshwater ecosystems in the basin.

CRediT authorship contribution statement

Carlotta Valerio: Conceptualization, Methodology, Formal analysis, Visualization, Writing - original draft. **Lucia De Stefano:** Conceptualization, Supervision, Funding acquisition, Writing - review & editing. **Gonzalo Martínez-Muñoz:** Methodology, Validation, Writing - review & editing. **Alberto Garrido:** Conceptualization, Funding acquisition, Writing - review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scitotenv.2020.141252.

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