

An ANN-Based Information System for Predictive Modeling of Green Antioxidant Extraction from Medicinal Plants

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Abstract

This paper presents an Artificial Neural Network (ANN)-based information system for predictive modeling of eco-friendly antioxidant extraction from local medicinal plants. The study combines laboratory extraction experiments with a data-driven machine-learning workflow in order to align the contribution with Artificial Intelligence, Computer Science Applications, and Information Systems. Four medicinal plant materials from the Sidi Bel Abbès region of Algeria were investigated: olive leaves, rosemary, pomegranate peels, and *Aloysia citriodora*. Experimentally, the work compared maceration, decoction, ultrasound-assisted extraction, and ultrasound-assisted extraction coupled with mechanical agitation. Phytochemical assays confirmed that ultrasound plus agitation produced the strongest overall extraction performance, especially for total phenolic content and antioxidant activity. To move beyond descriptive chemistry and toward intelligent decision support, a global ANN model was developed to predict DPPH inhibition using plant type, extraction technique, and extract concentration as input descriptors. The model was trained and assessed using 5-fold cross-validation on 180 replicate-level observations. The selected multilayer perceptron architecture, with two hidden layers (16 and 8 neurons), achieved strong predictive performance with $R^2 = 0.975$, $MAE = 2.28$, and $RMSE = 4.97$. These results show that the proposed ANN framework can accurately capture the nonlinear interaction between botanical matrix, extraction strategy, and concentration-dependent antioxidant response. From an information systems perspective, the proposed workflow acts as a compact decision-support layer that can guide green extraction screening and reduce trial-and-error experimentation. The study therefore contributes an ANN-oriented computational framing of medicinal-plant extraction that is more suitable for an AI-centered journal while preserving the environmental and phytochemical relevance of the original research.

Keywords: Artificial Neural Network; Artificial Intelligence; Computer Science Applications; Information Systems; DPPH prediction; green extraction; medicinal plants

Introduction

Natural antioxidants from medicinal plants are increasingly investigated in green process engineering because extraction efficiency, solvent demand, and antioxidant preservation are strongly governed by operating conditions. Among non-conventional techniques, ultrasound-assisted extraction (UAE) is widely recognized as a sustainable intensification strategy that

enhances cavitation, improves mass transfer, shortens extraction time, and often increases the recovery of phenolic antioxidants compared with conventional approaches [1], [2].

In plant-based antioxidant research, the DPPH assay remains one of the most widely used analytical tools for assessing radical scavenging performance and IC_{50} behavior because it is rapid, inexpensive, and compatible with comparative screening of plant extracts [3]. From a data perspective, such assays generate structured input-output relationships in which botanical matrix, extraction procedure, and concentration jointly determine the observed antioxidant response.

This type of multivariate structure is well suited to Artificial Intelligence and Computer Science Applications. In particular, Artificial Neural Networks (ANNs) are effective for supervised nonlinear regression because they can learn complex mappings directly from experimental data without requiring an explicit mechanistic model [4]. Recent reviews on bioactive-compound extraction report that ANN-based approaches frequently outperform classical polynomial response-surface models when the process contains strong interactions, nonlinear effects, or multiple coupled variables [5].

The relevance of ANN is even stronger when antioxidant behavior is concentration-dependent, as in DPPH inhibition profiling. Earlier machine-learning work already demonstrated that ANN can successfully estimate DPPH radical scavenging activity from experimental patterns, highlighting the suitability of ANN for antioxidant-response modeling beyond conventional statistical fitting [6]. In this sense, an ANN can be viewed not only as a predictive algorithm but also as a compact decision-support component within a laboratory information system.

The present study originates from an eco-responsible extraction study on four medicinal plant materials from the Sidi Bel Abbes region of Algeria: olive leaves, rosemary, pomegranate peels, and *Aloysia citriodora*. To better align the work with an AI-oriented journal, this manuscript reframes the contribution around a global ANN-based predictive information system. The phytochemical dataset is retained to interpret extraction quality, while the richer DPPH dataset is used to construct the main ANN task, in which plant type, extraction method, and concentration are used to predict antioxidant inhibition. The objective is therefore to combine green extraction evidence with an ANN-centered computational framework suitable for Artificial Intelligence, Information Systems, and Computer Science Applications.

Materials and Methods

Experimental acquisition and phytochemical dataset

The laboratory study considered four medicinal plant materials commonly used in the Sidi Bel Abbes region of Algeria: olive leaves (*Olea europaea*), rosemary (*Rosmarinus officinalis*), pomegranate peels (*Punica granatum*), and *Aloysia citriodora*. Four extraction routes were compared: maceration, decoction, ultrasound-assisted extraction, and ultrasound-assisted extraction combined with mechanical agitation.

The original experimental study included a broader phytochemical characterization comprising total phenolic content (TPC), total flavonoid content (TFC), condensed tannins, hydrolysable tannins, DPPH radical scavenging activity, and IC_{50} . In the present paper, these experimental measurements are retained as the scientific basis of the extraction study; however, Table 1 reports only TPC and IC_{50} because these two indicators provide a compact summary of extraction efficiency and antioxidant effectiveness. More specifically, TPC was selected as the main descriptor of phytochemical recovery, whereas IC_{50} was retained as the main descriptor of antioxidant strength. The ANN model itself was not trained on the full phytochemical block; instead, it was developed from the richer DPPH dataset, using plant type, extraction technique, and concentration as input variables and inhibition percentage as the prediction target. This distinction is important because the experimental phytochemical dataset supports the interpretation of extraction performance, while the DPPH dataset provides the larger and more suitable sample structure for machine-learning modeling.

Table 1. Experimental summary dataset used to interpret extraction performance.

Plant material	Technique	TPC (mg GAE/g)	IC ₅₀ (mg/mL)
Olive leaves	Maceration	165.35	5.658
	Decoction	351.18	4.274
	Ultrasound	365.35	4.203
	Ultrasound + agitation	804.72	2.970
Rosemary	Maceration	532.28	1.137
	Decoction	826.77	0.702
	Ultrasound	987.40	0.433
	Ultrasound + agitation	4135.43	0.107
Pomegranate peels	Maceration	2181.10	0.088
	Decoction	3875.59	0.078
	Ultrasound	4022.05	0.070
	Ultrasound + agitation	4379.53	0.040
Aloysia	Maceration	1510.24	0.469
	Decoction	2401.57	0.374
	Ultrasound	2982.68	0.226
	Ultrasound + agitation	3918.11	0.124

Construction of the ANN information system

To make the study methodologically appropriate for an AI-oriented journal, the ANN module was designed as the central computational element of the manuscript. The information system architecture contains four layers: experimental acquisition, feature engineering, ANN training and validation, and decision-support output. This architecture is illustrated in Figure 1 and is consistent with compact data-driven laboratory decision systems in which measured experimental variables are transformed into predictive recommendations.

The ANN task was formulated globally rather than separately by plant. A single model was trained on all studied plants and all extraction methods, while plant identity was explicitly encoded as an input feature. This strategy is appropriate when the objective is to learn the combined nonlinear effect of plant type, extraction technique, and concentration within one unified predictive framework.

The final ANN dataset was constructed from the DPPH assay because it provides a richer response surface than the averaged phytochemical dataset. Using the four plant types, four extraction methods, six concentration levels, and replicate measurements, the machine-learning table contained 180 replicate-level observations. Each record included plant type, extraction technique, extract concentration, measured absorbance, and computed DPPH inhibition percentage.

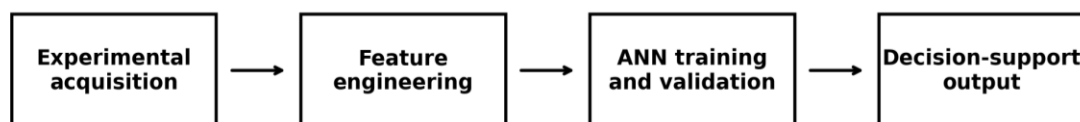


Figure 1. Four-layer information-system workflow used to transform laboratory measurements into an ANN-based predictive decision-support tool.

Feature engineering and ANN architecture

The input variables of the global ANN model were plant type, extraction technique, and extract concentration. Plant type and extraction technique were one-hot encoded, while concentration was standardized before training. The target variable was DPPH inhibition percentage. This formulation allows the ANN to learn concentration-dependent antioxidant behavior across

different plant-process combinations, rather than fitting a separate curve for each plant or each extraction route.

A feedforward multilayer perceptron was selected because it is a standard ANN architecture for tabular nonlinear regression and because MLP-type networks remain among the most widely used ANN configurations in extraction-process modeling [4], [5]. Several compact architectures were screened, and the best predictive compromise was obtained with two hidden layers containing 16 and 8 neurons, respectively. Rectified Linear Unit (ReLU) activation was used in the hidden layers, and the optimization was performed with the L-BFGS solver.

Model performance was assessed using 5-fold cross-validation with shuffling and a fixed random state. Three metrics were retained: the coefficient of determination (R^2), mean absolute error (MAE), and root mean square error (RMSE). This evaluation strategy was chosen to demonstrate predictive stability while reducing the risk of overinterpreting a single train-test split, which is particularly important in laboratory datasets of limited size [5].

Results and Discussion

Experimental trends supporting the ANN problem

The experimental results confirm that ultrasound-assisted extraction coupled with mechanical agitation delivered the strongest overall performance (Fig.1). For all four plant materials, the assisted process improved the recovery of total phenolics and reduced IC_{50} relative to maceration and decoction. This global trend is consistent with the UAE literature, where cavitation-assisted disruption of plant tissues enhances solvent penetration and mass transfer [1], [2]. It is also consistent with olive-leaf studies reporting higher phenolic and antioxidant recoveries under UAE than under conventional extraction [7].

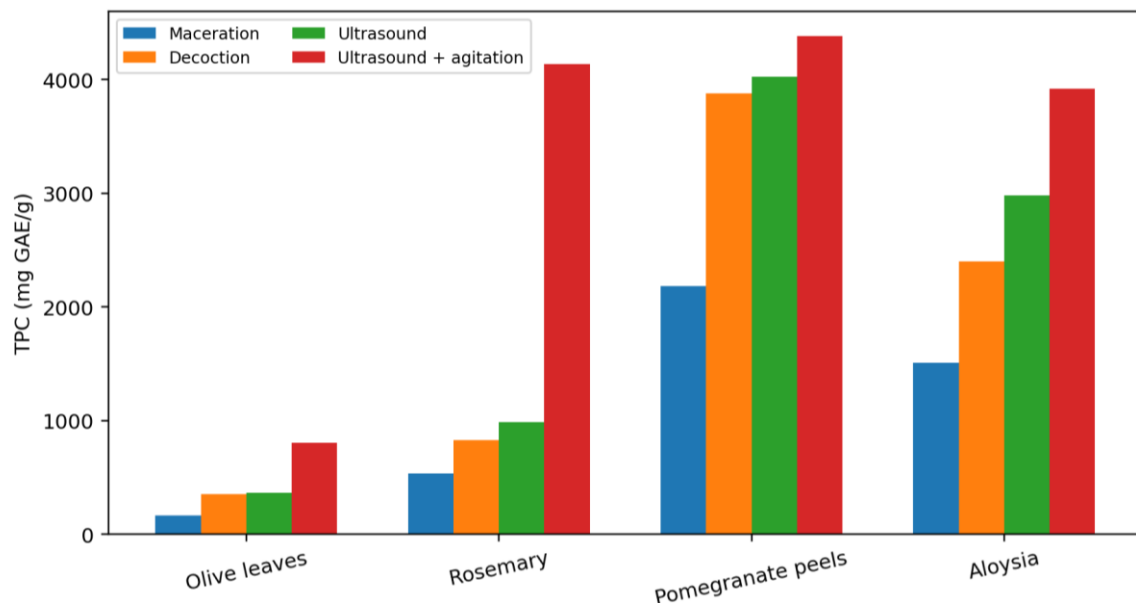


Figure 2. Total phenolic content by plant matrix and extraction technique.

The same intensification trend was reflected in antioxidant performance (Fig.2). IC_{50} values systematically decreased under ultrasound plus agitation, which indicates stronger radical scavenging behavior. For rosemary, our qualitative ranking agrees with recent work showing that ultrasonication-based techniques are among the most effective routes for maximizing rosemary polyphenols and DPPH-active compounds [8]. For pomegranate peel, the strong antioxidant performance observed here is in line with previous reports identifying pomegranate peel as a particularly rich matrix for ultrasound-enhanced phenolic recovery and antioxidant activity [9], [10]. Likewise, the *Aloysia citriodora* results agree with recent evidence showing

that ultrasonic extraction yields higher phenolic and flavonoid contents and lower IC₅₀ values than maceration-based extraction [11].

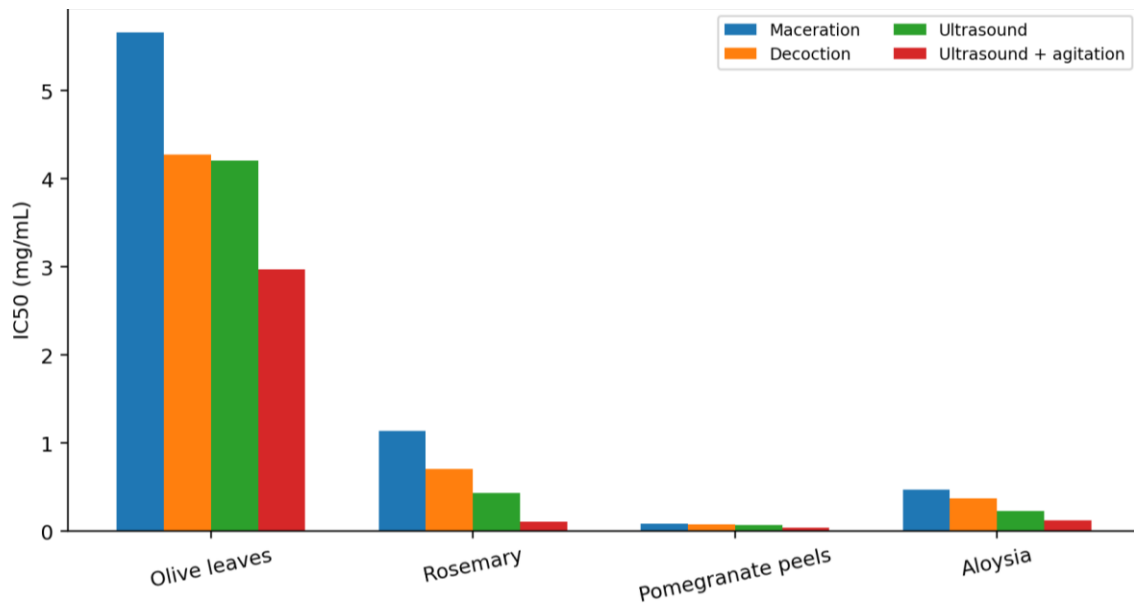


Figure 3. IC₅₀ values by plant matrix and extraction technique.

Although direct numerical comparison across studies must be made cautiously because solvent systems, extraction temperature, sonication power, and expression units differ, the bibliographic comparison supports the same overall conclusion: assisted extraction generally increases phytochemical recovery and improves antioxidant response. Therefore, the experimental block of the present work is well aligned with the broader green-extraction literature and provides a sound foundation for ANN-based modeling.

Performance of the global ANN model

The global ANN model achieved strong predictive performance in 5-fold cross-validation. Using plant type, extraction method, and concentration as inputs, the selected multilayer perceptron accurately reproduced the experimental DPPH inhibition response over the full dataset (Table 2).

The final cross-validated performance was $R^2 = 0.975$, MAE = 2.28, and RMSE = 4.97 (Fig.3). These values indicate that the ANN captured the dominant nonlinear structure of the antioxidant-response surface and that the residual prediction error remained low relative to the full inhibition range. In methodological terms, this performance is consistent with the recent literature showing that ANN models often provide more flexible and accurate extraction-process prediction than response-surface models when nonlinear interactions are prominent [5].

Our ANN results are also comparable to recent empirical studies in the field. For example, AI-assisted UAE optimization studies have reported excellent predictive accuracy for antioxidant-related responses, including yerba mate models with R^2 values above 0.99 for yield, TPC, and DPPH, and ANN-guided mustard-seed extraction models that improved predicted TPC, TFC, and DPPH responses under optimized UAE conditions [12], [13]. Unlike those studies, which optimized a single botanical source under designed experimental settings, the present work uses one global ANN to integrate multiple plant matrices, extraction methods, and concentrations within a single predictive framework.

Table 2. Cross-validated performance of the global ANN model.

Model	Observations	Inputs	Validation	R ²	MAE / RMSE
MLP (16, 8), ReLU, L-BFGS	180	Plant + method + concentration	5-fold CV	0.975	2.28 / 4.97

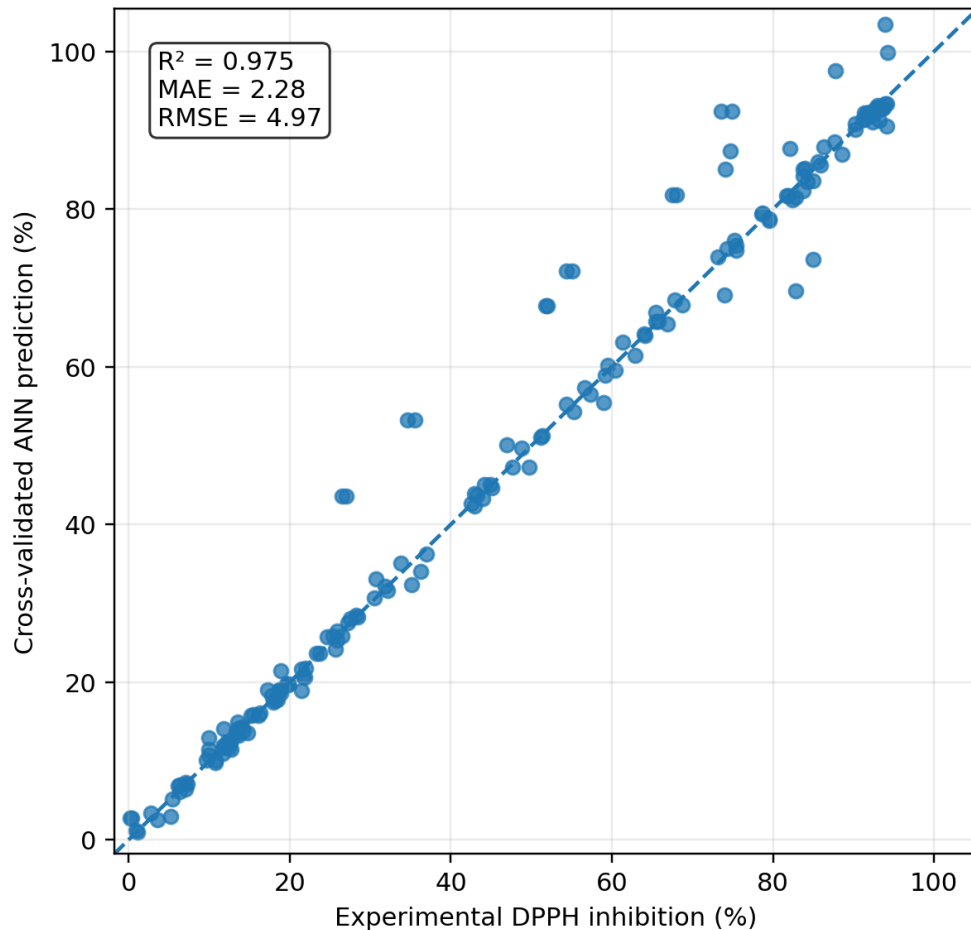


Figure 3. Parity plot comparing experimental DPPH inhibition with cross-validated ANN predictions.

ANN interpretation from a computer science and information systems perspective

From a computer science perspective, the ANN behaves as a nonlinear regression engine that maps mixed categorical-continuous descriptors to an experimentally measurable antioxidant response. The high R² indicates that the selected architecture is expressive enough to represent the combined influence of plant type, extraction route, and concentration without requiring a handcrafted mechanistic equation. This is coherent with the broader ANN literature in bioactive extraction, which highlights the ability of neural models to capture interactions that are difficult to describe through fixed polynomial formulations [4], [5].

From an information systems perspective, the model functions as a decision-support layer. Once the experimental descriptors are entered, the system can estimate inhibition behavior before full downstream analysis. This capability is useful for green extraction screening because it supports faster comparison of alternatives and reduces dependence on purely trial-and-error experimentation. In this sense, the proposed workflow can be interpreted as a

compact laboratory information system in which data acquisition, model inference, and extraction-route prioritization are linked in a single computational loop.

Scientifically, the use of a single global model is justified because the plant factor is explicitly included in the feature space. The model therefore does not ignore inter-plant variability; instead, it learns how that variability interacts with extraction technique and concentration. Separate plant-specific models may still be useful in future work, but the global model is more appropriate for a journal article centered on intelligent information systems because it provides one unified predictive framework.

Conclusion

This manuscript repositions an eco-friendly antioxidant-extraction study as an ANN-centered computational contribution. The laboratory experiments showed that ultrasound-assisted extraction coupled with mechanical agitation produced the most favorable phytochemical and antioxidant outcomes across olive leaves, rosemary, pomegranate peels, and *Aloysia citriodora*. Comparison with the literature confirms that these trends are consistent with published UAE studies on olive leaves, rosemary, pomegranate peel, and *Aloysia*.

The main methodological contribution of the paper is the construction of a global ANN-based information system that predicts DPPH inhibition from plant type, extraction technique, and concentration. The selected multilayer perceptron achieved a strong 5-fold cross-validated performance ($R^2 = 0.975$), demonstrating that the antioxidant-response surface can be modeled accurately within a compact ANN framework. This level of performance is consistent with recent ANN-based extraction studies and reinforces the relevance of ANN as a robust tool for AI-assisted green process optimization.

This AI-oriented framing makes the study substantially more suitable for a journal focused on Artificial Intelligence, Computer Science Applications, and Information Systems. The work now offers not only experimental extraction evidence but also a credible predictive module that can support intelligent screening and future digital decision support for green process engineering.

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