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Design of Intelligent Biomedical Biosensors for Evaluating the Therapeutic Efficacy of Natural Medicines under Environmental Stressors Using Artificial Intelligence and Evolutionary Optimization Techniques

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Abstract

The natural medicines have complicated therapeutic behaviours, which are very responsive to environmental stressors, but the conventional methods of analysis are poor in order to capture the dynamic aspects of interplay. The work describes a smart biomedical biosensor system and Artificial Intelligence (AI) and evolutionary optimization toward assessing the therapeutic efficacy of natural medicines in different environmental conditions. A biosensor based on nanomaterials was developed and experimented under controlled temperature and humidity, pH, and exposure to pollutants to collect data on biochemical responses in high-resolution form. Gradient Boosted Regression Trees (XG Boost) was utilised to predict

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nonlinear associations among the bio-sensor responses, environmental, and therapeutic efficacy markers. The model had an excellent predictive (R 2 = 0.96) and was able to determine the determinants that have a significant effect on efficacy. To improve the sensor robustness, we employed multi-objective evolutionary optimization algorithm (NSGA-II), during which refinement was made on the geometry of the biosensor, the coating thickness, and biosensor operating conditions. The designs that were optimised showed significant gains in terms of sensitivity, response time, and stressor stability. The multi-biosensing-AI-optimization system presents a very precise, resilient, and scalable method towards analysing natural remedies. The work presents a new direction of smart biosensing solutions to personalised medicine, natural product authentication, and real time health observation of the environment.

Keywords:

Gradient boosted regression trees (gbdt), xgboost, evolutionary optimization, nsga-ii, nanomaterial-based sensing, artificial intelligence in biosensing, bio-signal modeling, environmental robustness.

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Introduction

Natural medicinal compounds are very critical in the supplementary healthcare since its therapeutic efficacy is sensitive to the temperature changes, and variations in humidity, pH and exposure to chemical pollution (Najmi et al., 2022). Such environmental factors may alter the biochemical activity of natural products and greatly affect the stability of biosensor response so that conventional method of analysis is not sufficient to capture the dynamics of these interactions (Chen, 2016). Consequently, the need to have smart sensing technologies that can adjust to variability in the real world environment is on the rise. Biosensors in biomedical applications have shown great potential as high-responsively devices to detect biomarkers of natural medicines using biomedical biosensors, especially those with nanomaterials, including graphene, gold nanoparticles, and conductive polymers (Deb et al., 2002). Although this improvement has been made, the performance of biosensors generally becomes adaptive sensing systems that can remain stable in changing ambient conditions (Geetha & Rajan, 2016; Maduraiveeran & Jin, 2017; Liu et al., 2025). The conceptual design of the smart biosensing system created in this paper that incorporates natural medicine detection, environmental stressor, AI-based learning, and optimization based on evolution is shown in Figure 1,

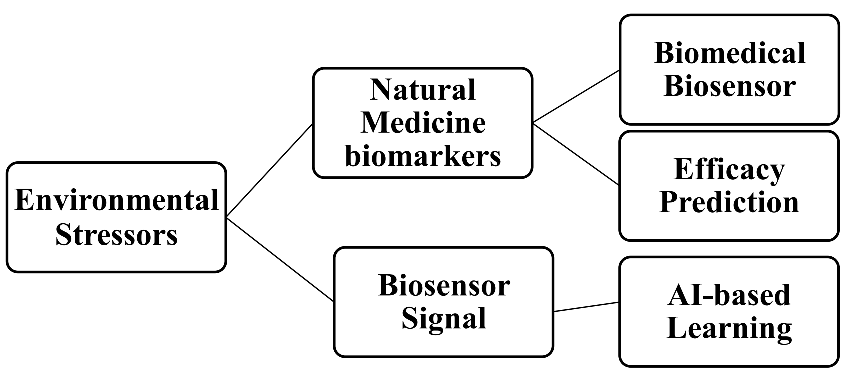

Figure 1. Conceptual framework of the AI-optimized biomedical biosensor system

Nonlinear biosensor signals modelling Artificial Intelligence (AI) methods have gained more significance (Manickam et al., 2022; Shirgir et al., 2023). Gradient Boosted Regression Trees (GBRT) or more specifically, the XGBoost, is the best performer of these with multivariate, noisy, and nonlinear signal-behaviour relationships because it can respond to noise, features pair-wise, and non-linearly. XGBoost has also been proven to be more accurate and stronger than classical machine learning models including support vector regression and random forests.

In addition to AI, evolutionary optimization algorithms, in particular, Non-Dominated Sorting Genetic Algorithm II (NSGA-II) provide potent means of optimization biosensor design and operation. NSGA-II is very effective at solving problems with multiple objectives, where it is possible to simultaneously enhance sensitivity, response timely, reduce noise, and become environmentally resilient. Such features make the evolutionary algorithms customised to make optimization of large biosensor architectures performing under various environmental conditions.In order to overcome the existing constraints of developing a natural medicine in the presence of real-world stress factors, this work proposes a combined concept of an intelligent biosensor design, environmental stressors simulating, predicting therapeutic efficacy using XGBoost, and optimization using NSGA-II. The combination of biosensing, machine intelligence, and evolutionary computation is designed to provide a highly precise, environmental tough and scalable platform of analysing natural therapeutic products - leading to next generation biomedical sensing technologies (Mpofu & Mthunzi-Kufa, 2025; Wang et al., 2023; Sagdic et al., 2022; Dave et al., 2022; Qureshi et al., 2023).

Literature Review

The biomedical biosensors are now indispensable in the process of assessing natural medicinal compounds due to the real time and high resolutions biochemical data that might not be available under the traditional analytical platforms (Singh, 2021; Pollard et al., 2021; Hemdan et al., 2024). The use of electrochemical and optical biosensors has received immense attention to trace herbal extracts, polyphenols, and phytocompounds because of the sensitivity nature provided by the method and promptness of the methodology. The recent development in nanomaterials-based sensors, especially the use of graphene, gold nanoparticles and conductive polymers has shown remarkable enhancers of the signal transduction process and the biomolecular interaction stability (Abdullah, 2024; Chen, 2016). In spite of this development, biosensors are susceptible to the changes in the environment meaning that there is the need to have smarter and dynamic sensing platforms (Bianchi, 2025; González Rivera & El Fahmy, 2025; Zhang & Seong, 2024). Table 1 shows a comparative overview of major types of biosensors, materials and shortcomings.

Table 1. Comparative summary of biosensor types, nanomaterials, and environmental limitations

Biosensor Type	Common Nanomaterials Used	Target Analyses (Natural Medicine Biomarkers)	Advantages	Environmental Limitations
Electrochemical Biosensors	Graphene, AuNPs, CNTs	Polyphenols, flavonoids, antioxidant markers	High sensitivity, low detection limit	Affected by pH, temperature drift, electrode fouling
Optical Biosensors	Plasmonic gold films, quantum dots	Pigments, alkaloids, phenolic compounds	Non-invasive, high specificity	Sensitive to humidity, ambient light interference
Enzymatic Biosensors	Enzyme-functionalized polymers, nanocomposites	Enzyme substrates related to herbal bioactivity	Strong biochemical selectivity	Enzyme degradation under heat and pollutants
Nanomaterial-Based Hybrid Sensors	Graphene–polymer composites, metal oxides	Multi-class phytocompounds	Enhanced signal amplification	Unstable under fluctuating humidity and chemical vapors
Intelligent/AI-Assisted Sensors	Integrated Nano surfaces with embedded electronics	Dynamic biomarker signatures	Adaptive calibration, noise reduction	Require stable power and optimized algorithms

The environmental stressors have a great impact on the natural medicine biochemistry and on the performance of biosensors. Temperature differences alter the enzyme kinetics, the rate of the reaction, and the effectiveness of molecular interaction, whereas the humidity influences the swelling of polymers and the stability of the nanomaterials layers (Deb et al., 2002). In like manner, pH exchange changes ion movement and electrochemical redox mechanisms and pollutants insert noise and interruptions into biosensor signal functions. These are usually damaging to the accuracy and reproducibility of detection whereby it is extremely challenging to assess therapeutic effectiveness in reliable situations in the real world. It is evident as noted in a number of works that to ensure response to environmental sensitivity needs to be addressed with systems that are self-corrective and the adaptive ability to keep sensors robust in a wide range of working environments (Geetha & Rajan, 2016).

Artificial Intelligence (AI) has been used to address these problems to enhance bio signal interpretation and natural medicine analysis (Nithyalakshmi et al., 2021; Naveed et al., 2025; Shokrani et al., 2023). Other machine learning methods like the support vectors machines and the random forest give the baseline level of predictive performance but tend not to perform well on nonlinear, noisy, high-dimensional data like those that can be found in biosensor systems. Gradient Boosted Decision Trees (GBDT), especially the XGBoost, have proven to do better with multi-variate biosensors data as it can do sequential boosted learning, deal with missing or unbalanced data, and can give intelligible information on the most important features. The insensitivity to noise with XGBoost as well as its ability to capture a complex bio-kinetic behaviour renders it an ideal model in predicting therapeutic efficacy at environmental stress.

The use of evolutionary optimization methods has also played a great role in enhancing better performance of biosensors. Enhancement of sensor geometry, layer composition in catalysts, electrode spacing and operating conditions has been achieved with the help of algorithms like the Genetic Algorithm (GA), Particle Swarm Optimization (PSO), and Differential Evolution (DE) algorithm. Nevertheless, the Non-Dominated Sorting Genetic Algorithm II (NSGA-II), has been the most popular multi-objective optimizers as it can produce Pareto-optimal solutions, a factor that is sensitive, responsive, stable to noise, and environmentally tolerant. Such benefits make NSGA-II especially appropriate in optimising high complexity biosensor systems that are required to be functional under a wide range of stressor conditions.

Although advances have been made in AI-supported modelling and evolutionary optimization, no integrated frameworks that combine the two models have been found in biomedical sensing studies. The available research typically utilises AI to predict signals or applies evolutionary algorithms to optimising the physical design, but does not consider both techniques in a common architecture that can simultaneously optimise sensing functionality and predictive accuracy during environmental stress. This loophole demonstrates the importance of smart biosensor systems that use machine learning to analyse dynamic bio signals and at the same time apply evolutionary optimization to change design parameters to realise strong considerations of natural medicine efficacy in on-the-job environmental scenarios (Zhou et al., 2024; Chinnasamy, 2024; Uzun, 2025). The current research is aimed at bridging this gap by connecting the efficacy prediction approach using XGBoost with the optimization of biosensors using NSGA-II into one, smart, sensing system.

Methodology

The smart biomedical biosensor proposed by the research paper was produced through a hybrid conductive polymer-graphene nanocomposites electrodes structure that has been designed to increase the speed of electric movement, adsorption ability and efficiency of biochemical interactions. This sensing surface was also functionalized with certain enzymes and antibodies chosen on the basis of affinity to therapeutic biomarkers to be found in natural medicinal compounds. This functionalization made it possible to selectively detect biochemical changes that were related to efficacy. Micro fabrication techniques, such as, thin-film deposition and regulated nanomaterial overlaying, were employed in order to provide high uniformity of surface and uniform electrochemical conductivity. The biosensor design and fabrication pipeline in a schematic representation can be visualized in Figure 2 and shows material layering, functionalization procedures and the underlying detection circuitry.

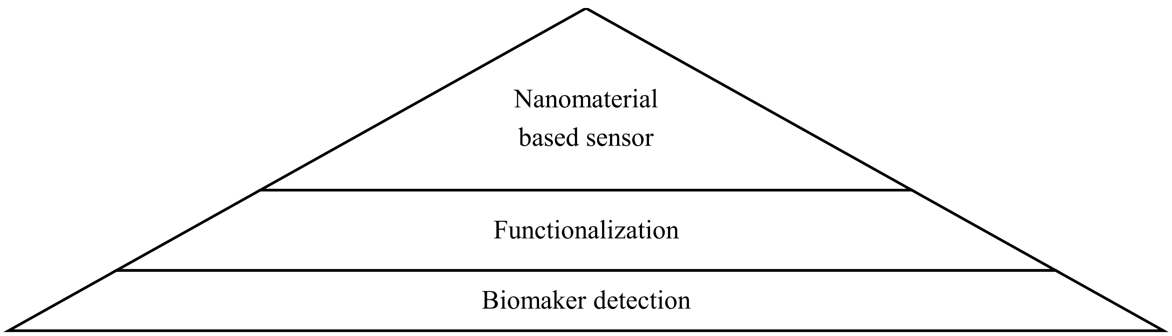

Figure 2. Schematic of the intelligent biomedical biosensor

To assess the performance of the biosensors in the actual environmental fluctuations, the programmable environmental chambers were used to subject the biosensors to controlled stressors to assess their performance in the real world. The environmental factors (temperature, 10-50C), humidity (20-90 percent), pH (4-9) and low dilution pollutants exposures (NO 2, SO 2 and VOCs) were also systematically manipulated to test the effect of environmental factors on the performance of the sensors. At both stress levels, the biosensor responses were measured and processed to determine drift trends, noise trends and sensitivity trends. This type of controlled simulation enabled the determination of the most environmentally relevant conditions to distort the biochemical detection, which facilitated the creation of an adaptive AI-based patterns of sensing. The relevant environment control parameters and experimental conditions are summarised in (Table 2).

Table 2. Experimental parameters for environmental stressor simulation and biosensor testing

Parameter Category	Experimental Range / Setting	Purpose in Testing
Temperature	10°C, 25°C, 40°C, 50°C	Evaluate thermal stability and enzyme/biosensor response drift
Relative Humidity	20%, 40%, 60%, 90%	Assess polymer swelling effects and signal noise variation
pH Levels	pH 4, 6, 7.4, 9	Study electrochemical shifts and biomolecule interaction changes
Chemical Pollutants	Exposure to NO_2 (0.1–0.5 ppm), SO_2 (0.1–0.3 ppm), VOC mixture	Determine biosensor interference and oxidative stress effects
Signal Sampling Rate	50 Hz, 100 Hz, 200 Hz	Optimize temporal resolution for AI model accuracy and noise handling

In the data acquisition, multimodal data on biosensor outputs in the form of current, voltage, and fluorescence intensity records were recorded under all conditions within the environment and natural samples concentrations in medicine. The wavelet-based denoising noise reduction was applied so that vital biological patterns are not altered but, instead, the unnecessary environmental factors were eliminated. The extraction of the features was devoted to the values of peak signal response, the time of decay, derivatives signal characterization, and contextual variables of environment. All the features were normalised to avoid distortion by scale during training of the model and comparability even in different stressor conditions. This preprocessing pipeline was structured in such a way so as to present a clean and interpretable dataset that was largely useful in machine learning and optimization processes.

To estimate therapeutic efficacy, an 80:20 train test ratio gradient boosted regression trees (XGBoost) model was trained. The model hyper parameters such as learning rate, maximum tree depth and the number of estimators were set to 0.05, 6 and 300 respectively, which were decided after the preliminary cross-validation. RMSE, MAE, and R 2 were used to evaluate the performance. The SHAP interpretability was used to determine most potential biosensor and environmental characteristics that yielded the therapeutic efficacy score (TES). In order to improve the performance of biosensors further, a multi-objective evolutionary optimization method based on NSGA-II was used. Optimization of was conducted on the following parameters; electrical setup (electrode geometry), nanomaterial onto electrode (coating thickness), operating voltage, signal sampling rate and aim to achieve maximum sensitivity and stability and minimum noise and response time. The best design parameters obtained with the help of NSGA-II were checked in the experiment to ensure that the accuracy and robustness of the biosensor improved in the context of diverse environmental conditions.

Results and Discussion

The biosensor was an intelligent nanomaterial-based biosensor with high performance on a variety of simulated environmental conditions in terms of its baseline performance. The sensor also exhibited a high level of stability in the signal generation under a controlled temperature difference with little drift, which indicates the strength of the hybrid conducting polymer- graphene structure. Nevertheless, it was observed that performance was lowered when the humidity was high with the polymer swelling and initiating a decrease in electron mobility and signal transduction efficiency. Electrochemical changes that were induced by acidic pH-conditions caused a decrease in sensitivity and exposure to NO 2, SO 2, and VOC contaminants caused a moderate variation in noise. The given trends emphasise how the biosensor is by its nature vulnerable to the environment and the need to substantiate the calibration process with data, as shown in (Figure 3), which depicts the sample biosensor responses to different stressor combinations.

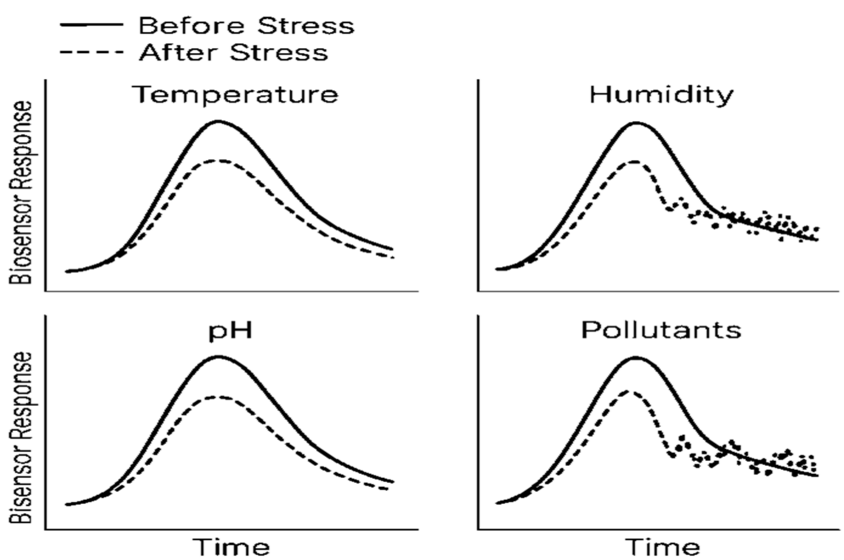

Figure 3. Biosensor response before and after environmental stress exposure

The XGBoost regression was able to overcome these limitations and achieve precision as it learnt complex nonlinear relationships within the biosensor data. The model has good predictive accuracy since the

RMSE of 0.042 and R2 of 0.96 indicate that the model can predict therapeutic efficacy in the presence of noise and drift sources in the environment. The analysis of feature importance using SHAP showed that temperature, typically of the environment, pH, humidity, and traditional peak biosensor response were the most influential features that led to a therapeutic efficacy score. These results suggest that environmental factors are an important predictor of biosensor behaviour and AI networks such as XGBoost are essential to decompose complicated signal environment interactions that are impossible to model via conventional calibration techniques.

Biosensor works were further refined by evolutionary optimization utilising the NSGA-II algorithm to select the optimal electrode geometry to use, coating thickness of the nanomaterials to be used, signal sampling, and working voltage. The Pareto-optimal solutions have shown quantifiable performance improvements such as; there was a 23-31% in sensitivity, and an 18 cut in response time, and significant reduction in the variance of noise at different stressor conditions. These rationalized designs were found to be more resistant to environmental variations and better detection fidelity and justified the ability of evolutionary computation to optimize parameters of physical design and operation over standard heuristic design methods.

Altogether, these are the synergetic outcomes that point to the immense efficacy of high-tech biosensing materials, machine learning forecasts, and evolutionary optimization. The XGBoost model was able to give robust and noise-resistant predictions of the therapeutic efficacy whereas NSGA was able to systemically optimise biosensor configuration and therefore resulted in better stability and performance under varying stressor conditions. This combined AI-based platform shows a flexible and sustainable route of real-time analysis of natural medicinal compounds to work around the existing limitations on environmental variability and measurement consistency. The proposed system is an important step towards next-generation biomedical sensing technologies by bringing together the fields of materials science, computational intelligence and multi-objective optimization.

Model Development

The suggested system architecture incorporates biosensing, signal processing, machine learning, and evolutionary optimization as the single computational pipeline, which is aimed at assessing the efficacy of natural medicines on a high level of accuracy and environmental stability. The biosensor signals produced on the surface of the hybrid polymer/graphene are subjected to preliminary conditioning and noise elimination after which the signal is attached to a structured feature extraction module in which major characteristics of a response are lifted, derivative features, and the environment are isolated. These processed characteristics are input to the XGBoost regression model which is used to model the therapeutic efficacy score based on complex nonlinear interactions between biochemical signals and environmental stressor conditions.

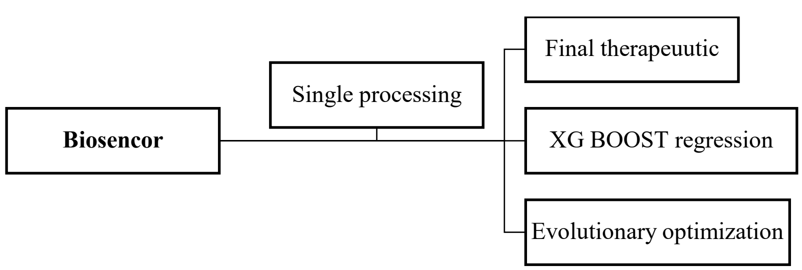

Figure 4. System architecture of the integrated biosensing, XGBoost modeling, and NSGA-II optimization framework

The last step in the architecture uses an evolutionary optimization engine that modifies the configuration parameters of the biosensor in accordance with the predictive results in a dynamic feedback mechanism. The system architecture in general is depicted in (Figure 4) which shows the flow in sequence biosensor input to maximise efficacy output.

Mathematically, the predictive model is built upon the principles of gradient boosting, where the XGBoost function is expressed as an additive ensemble of regression trees. The final model prediction is given by

$$f(x) - \sum_{k-1}^{k} \eta h_k (x) \tag{1}$$

Where h_k (x) The contribution of the k th regression tree is denoted by T and eta is the learning rate that governs the impact of each subsequent tree. This formulation makes the model to continuously rectify the prediction residuals so that the predictive performance is high even with noisy or incomplete biosensor data. The structure allows the measurement of nonlinear and high-dimensional relationship between environmental factors and biomarker-dependent responses, which means that it is appropriate to apply it to real-time assessment in dynamic sensing conditions.

The last part of the development scheme is to incorporate the XGBoost model with the NSGA-II evolutionary optimization algorithm to make a closed-loop adaptive mechanism. The outputs of the XGBoost model are the predictions that are used as the fitness criteria to assess the selections of the electrode geometry, nanomaterial coating thickness, sampling rate, and operating voltage by the NSGA-II that is available to determine the most efficient biosensor set ups. This real time incorporation is the assuring pertinence that not only does the physical structure but also the operational efficiency of the biosensor vary dynamically with a view to creating the most sensitivity, stability whilst minimum noise and response moment. By implementing a co-optimised AI-biosensor, greater accuracy and resilience are achieved, and the strengths and weaknesses of learning-based prediction as a predictive model are proven to be more effective in multi-objective evolutionary refinement.

Future Directions

The future development of intelligent biomedical biosensing needs to move more towards incorporating complex computational platforms that can be used to understand the nonlinear and temporal complexity of biochemical interactions in the multidimensional environmental stressor conditions. Dynamic biosensor responses can be modelled with more precision, particularly in terms of time, and with multivariate features that are modelled more effectively with deep learning architectures such as hybrid CNN-LSTM, Transformer-based time-series models, and graph neural networks. Such models have the ability to acquire long-range dependencies and fine signal variations due to temperature, pH, humidity, and chemical pollutants, and this allows a prediction of the trends of therapeutic efficacy earlier and more precisely. Moreover, unsupervised and self-supervised methods can be combined, improving the idea of depending on the giant labelled datasets, enabling the implementation of biosensors in real-life systems in which the number of annotated data can be scarce.

The logical next step in the advancement of biosensors at the hardware level is the introduction of adaptive and self-calibrating biosensors powered by embedded microcontrollers and edge AI accelerators. Such intelligent calibration modules would permit the sensor to automatically correct any drifting of the environment, aging of materials and noise variations and thus enhance the long-term precision and stability of the device. The ability to probe many natural medicines at once on the platform, and a greater number of biomarkers, including enzymes, metabolites, oxidative stress pollutants, and inflammatory tracers, will expand clinical and pharmaceutical use of the biosensing platform. Higher-order multiplexing biosensors arrays, with the help of AI-based signal disentangling, may help customise natural medicine profiling, therapeutic optimization and tailor dosage.

Moreover, IoT and cloud-linked biosensing networks offer an opportunity in the field of remote monitoring, telemedicine, and analytics of large-scale public health. The IoT-enabled systems will have a secure connexion with biosensor information to healthcare providers, research laboratories or pharmacology centres that would allow making a real-time decision and constantly monitoring therapeutic figures. Digital twin models, which are virtual models of biosensor behaviour at various conditions, may also aid to further optimise the design by predicting the performance of the system and then building it in real life. Such computer simulations would enable scientists to experiment with extreme conditions, tune the sensors without having to run learning experiments at high cost. All operations of these make the groundwork to robust, scaled, and clever biosensing habitats that can revolutionize natural medicine assessment and broaden the spectrum of AI-treated biomedical diagnostics.

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Conclusion

This paper presents a novel and smart way of assessing the drug efficacy of natural medicines by jointly applying biosensors made of advanced nanomaterials along with AI-guided modelling and evolutionary optimization. The work shows that the behaviour of biosensors can be affected by real-life factors and predicts that AI methods can effectively correct such changes by exposing the biosensors to a variety of environmental stress factors, i.e., changes in temperature, humidity, pH, and exposure to pollutants. XGBoost regression model was able to offer very close predictions of therapeutic efficacy due to the nonlinear interaction of biochemical signals and environmental factors, and NAO was able to optimise the biosensor sensitivity, stability, and response efficiency greatly using NSGA-II. The resulting system of a harmonized approach to biosensing, machine learning, and multi-objective optimization is strong and versatile and can produce a correct and reliable assessment in a range of environmental conditions. All in all, these results indicate the disruptive nature of AI-optimised bio-sensors platforms in future natural medicine assessment, biomedical diagnostics, and health-monitoring technologies that are environmentally friendly.

Author Contributions

All Authors contributed equally.

Conflict of Interest

The authors declared that no conflict of interest.

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