Artificial Intelligence-Based Prediction of Antibacterial and Immunological Effectiveness of Bacterial Cellulose-MXene Biocomposites

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Abstract: Background. Acute purulent infections are characterized by high microbial burden, immune dysregulation, and delayed tissue repair, leading to unpredictable treatment outcomes. Bacterial cellulose-based biomaterials, particularly BC-MXene biocomposites, demonstrate promising antibacterial and immunomodulatory properties; however, their effectiveness depends on complex interactions between microbiological, immunological, and reparative factors. Artificial intelligence (AI) algorithms offer new opportunities to integrate multidimensional experimental data and predict therapeutic effectiveness. Objective. To evaluate the use of artificial intelligence algorithms for predicting the antibacterial and immunological effectiveness of BC-MXene biocomposites in experimental models of acute purulent infection. Materials and Methods. An experimental study was performed on outbred white rats with mixed-etiology purulent infection induced by Staphylococcus aureus, Escherichia coli, and Pseudomonas aeruginosa. Animals were divided into three groups receiving BC-MXene biocomposite dressings, bacterial cellulose-only dressings, or conventional local therapy. Microbiological dynamics, immune response indicators, cytokine trends, and morphological healing parameters were assessed over 14 days. Experimental data were digitized and analyzed using supervised AI algorithms, including logistic regression, random forest, and gradient boosting models, to predict treatment effectiveness. Results. BC-MXene treatment resulted in faster bacterial load reduction, improved immune response normalization, and accelerated tissue repair compared with control groups. By day 14, bacterial load decreased to 3.2×10^2 CFU/ml in the BC-MXene group compared with 1.0×10^3 CFU/ml in the bacterial cellulose group and 4.5×10^3 CFU/ml in the control group. The best-performing machine learning model (gradient boosting) achieved 93.5% accuracy and an AUC of 0.96. Conclusion. AI-based analysis provides an effective framework for predicting the antibacterial and immunological efficacy of BC-MXene biocomposites. The integration of advanced biomaterials with artificial intelligence enhances the objectivity and precision of experimental evaluation and supports future translational applications in purulent infection management.

1 INTRODUCTION

Acute purulent infections remain one of the most complex and unresolved problems in modern clinical medicine and surgery due to their high prevalence, polymicrobial etiology, prolonged inflammatory course, and frequent development of local and systemic complications [1]. Despite the availability of modern antimicrobial agents and advanced surgical techniques, the incidence of unsatisfactory treatment outcomes remains high, largely because conventional therapeutic strategies often fail to adequately address the combined effects of microbial persistence, immune dysregulation, and impaired tissue repair.

This complexity is particularly evident in mixed-etiology infections caused by Gram-positive and Gram-negative pathogens, where microbial synergy and biofilm formation further reduce treatment predictability [2], [3].

In recent years, increasing attention has been directed toward the development of advanced biomaterials for local wound management as an alternative or adjunct to systemic antimicrobial therapy. Among these materials, bacterial cellulose (BC), synthesized by *Komagataeibacter xylinus*, has gained considerable interest due to its unique physicochemical and biological properties, including high porosity, excellent water retention capacity, mechanical stability, biocompatibility, and absence of allergenic effects. These characteristics make BC an effective wound dressing material capable of maintaining an optimal moist environment, absorbing exudate, and supporting tissue regeneration [4], [5].

The integration of nanotechnology into BC-based systems has further expanded their therapeutic potential. MXene nanomaterials, belonging to a class of two-dimensional transition metal carbides and nitrides, exhibit pronounced antibacterial activity through mechanisms such as bacterial membrane disruption and induction of oxidative stress. When incorporated into BC matrices, MXene enhances antimicrobial efficacy while preserving the favorable structural and biological properties of bacterial cellulose [6]. Experimental studies have demonstrated that BC-MXene biocomposites possess not only antibacterial activity but also immunomodulatory and reparative effects, making them promising candidates for the local treatment of purulent infections [7].

However, the biological effectiveness of BC-MXene biocomposites depends on a complex interaction of multiple variables, including bacterial load dynamics, immune response intensity, cytokine balance, and tissue repair processes. Traditional statistical methods often provide limited insight into these nonlinear and multidimensional relationships, reducing the ability to accurately predict treatment outcomes. In this context, artificial intelligence (AI) algorithms represent a powerful analytical tool capable of processing large heterogeneous datasets, identifying hidden patterns, and generating predictive models with high accuracy [8].

The application of AI in biomedical research enables the integration of microbiological, immunological, and morphological data into unified predictive frameworks. Such approaches are particularly valuable for evaluating multifunctional biomaterials, where therapeutic effects cannot be adequately described by a single parameter [9], [10]. AI-based prediction of antibacterial and immunological effectiveness may improve experimental interpretation, support personalized treatment strategies, and optimize translational pathways from laboratory research to clinical practice.

Therefore, the present study focuses on the use of artificial intelligence algorithms to predict the antibacterial and immunological effectiveness of BC-MXene biocomposites in experimental models of acute purulent infection, representing a convergence of biomaterials science, immuno-microbiology, and digital health technologies.

2 RESEARCH OBJECTIVE

The objective of this study was to evaluate the feasibility and effectiveness of using artificial intelligence algorithms to predict the antibacterial and immunological efficacy of BC-MXene biocomposites in experimental models of acute purulent infection.

3 MATERIALS AND METHODS

This study was conducted as a comprehensive experimental investigation combining microbiological, immunological, morphological, and computational approaches. The experimental model was developed using three-month-old outbred white laboratory rats weighing 160-180 g, selected for their reproducible immune and wound-healing responses. Animals were maintained under standard vivarium conditions and all procedures were performed in accordance with ethical guidelines for experimental research.

4 ARTIFICIAL INTELLIGENCE MODELING PIPELINE

All experimental data were converted into a structured dataset suitable for machine learning analysis. The dataset comprised 60 observations in total (one per animal, n = 60), with each experimental subject (rat) represented as a single observation, while temporal biological measurements were aggregated and included as predictive features.

The following input features were used for model development:

- Bacterial load (CFU/ml) on days 3, 7, and 14.
- Serum levels of pro-inflammatory cytokines (IL-6, TNF-α).
- Phagocytic activity index of neutrophils (%).
- Leukocyte count (10^9/L).
- Granulation tissue maturity score.
- Epithelialization score.
- Angiogenesis score.
- Time-to-bacterial-clearance indicator.

Prior to model training, data preprocessing included normalization of continuous variables using z-score scaling, detection and removal of extreme outliers using the interquartile range (IQR) method, and imputation of occasional missing values by median substitution.

Machine learning models were implemented using the Scikit-learn library (version 1.3.2, Python 3.11). Hyperparameter optimization was performed using grid search combined with cross-validation.

Model validation employed repeated stratified cross-validation (5×10-fold) to ensure robust internal validation and maintain class distribution in each fold. Random seeds were fixed (seed = 42) to ensure reproducibility.

The following hyperparameters were optimized:

1) Logistic regression:
   - penalty = L2.
   - C = 0.1-10.
2) Random forest:
   - number of trees = 100-500.
   - max depth = 5-15.
3) Gradient boosting:
   - learning rate = 0.01-0.1.
   - number of estimators = 100-300.
   - max depth = 3-6.

Model performance was evaluated using accuracy, sensitivity, specificity, F1-score, and the area under the ROC curve (AUC).

Acute purulent infection was induced by inoculating standardized suspensions of *Staphylococcus aureus*, *Escherichia coli*, and *Pseudomonas aeruginosa* into soft tissues, reflecting a clinically relevant mixed-etiology infection model. Following confirmation of infection establishment, animals were divided into treatment groups receiving BC-MXene biocomposite dressings, bacterial cellulose-only dressings, or conventional local therapy.

Microbiological assessment included serial quantitative cultures of wound exudate with calculation of colony-forming units (CFU/ml), allowing dynamic evaluation of antibacterial effects. Immunological evaluation comprised measurement of humoral immunity indicators, non-specific defense factors, and cytokine profiles using enzyme-linked immunosorbent assays. Hematological parameters were analyzed to characterize systemic inflammatory responses, while histological examination of infected tissues was performed to assess inflammation resolution, granulation tissue formation, angiogenesis, and epithelialization.

All experimental data were digitized and structured into a unified dataset. Artificial intelligence modeling was implemented using supervised machine learning algorithms, including logistic regression, random forest, and gradient boosting models. Input features included microbiological load, immune markers, cytokine levels, hematological indices, and temporal parameters. Model training and validation were performed using cross-validation techniques to minimize overfitting. Predictive performance was evaluated using accuracy, sensitivity, specificity, and area under the receiver operating characteristic curve (AUC).

All experimental procedures were approved by the Institutional Animal Ethics Committee of Bukhara State Medical Institute (Protocol No. 6/2025, approved March 2025) and were conducted in accordance with international guidelines for the humane treatment of laboratory animals.

5 RESULTS

The experimental workflow integrated biological experimentation with AI-driven data analysis, enabling both descriptive and predictive evaluation of BC-MXene biocomposite effectiveness. Animals were monitored longitudinally, and treatment responses were systematically recorded and analyzed.

Equal group sizes ensured balanced datasets for AI model training and comparison. Uniform data collection across groups allowed algorithmic learning to focus on treatment-related differences rather than sampling bias (Table 1).

Statistical significance was set at $p < 0.05$ BC-MXene treatment resulted in the most rapid decline in bacterial burden. AI models identified early CFU reduction between days 3 and 7 as a strong predictor of favorable outcomes, highlighting the importance of early antibacterial response (Table 2).

Table 1: Experimental group distribution and data acquisition framework.

Group	Number of animals	Treatment modality	Data collected
I	20	BC-MXene biocomposite	Microbiological, immunological, morphological
II	20	Bacterial cellulose only	Microbiological, immunological, morphological
III	20	Conventional therapy	Microbiological, immunological, morphological

Table 2: Dynamics of bacterial load reduction (CFU/ml).

Day	BC-MXene	BC only	Control
3	4.0×10^5	6.7×10^5	9.1×10^5
7	1.1×10^4	3.5×10^4	8.0×10^4
14	3.2×10^2	1.0×10^3	4.5×10^3

Table 3: Quantitative immunological indicators during treatment.

Parameter	BC-MXene	BC only	Control
IL-6 (pg/ml) Day 3	72.4 ± 8.3	85.1 ± 9.6	97.3 ± 11.2
IL-6 (pg/ml) Day 14	28.6 ± 5.2	42.7 ± 6.1	61.9 ± 7.4
TNF-α (pg/ml) Day 3	65.2 ± 7.5	78.3 ± 8.4	90.7 ± 10.1
TNF-α (pg/ml) Day 14	24.9 ± 4.6	37.8 ± 5.2	54.3 ± 6.5
Phagocytic activity (%)	69.3 ± 6.4	58.7 ± 5.1	47.2 ± 4.8
Leukocyte count (10^9/L)	8.9 ± 1.2	10.7 ± 1.4	12.8 ± 1.6

Table 4: Histological and morphological healing scores (0-3 scale).

Indicator	BC-MXene	BC only	Control
Inflammation score	0.8 ± 0.4	1.5 ± 0.5	2.3 ± 0.6
Granulation tissue maturity	2.7 ± 0.3	2.1 ± 0.4	1.4 ± 0.5
Angiogenesis score	2.5 ± 0.4	2.0 ± 0.4	1.3 ± 0.4
Epithelialization score	2.8 ± 0.2	2.2 ± 0.3	1.5 ± 0.4

Table 5: Performance of AI prediction models.

Model	Accuracy (%)	Sensitivity (%)	AUC
Logistic regression	82.4	80.1	0.86
Random forest	91.2	89.7	0.94
Gradient boosting	93.5	92.1	0.96

Statistical significance was set at $p < 0.05$. BC-MXene treatment was associated with significantly lower levels of pro-inflammatory cytokines compared with both comparison groups ($p < 0.05$). The decline in IL-6 and TNF-α levels by day 14 indicates normalization of the inflammatory response. In parallel, phagocytic activity of neutrophils increased significantly in the BC-MXene group, suggesting enhanced innate immune defense and more efficient bacterial clearance. (Table 3).

Histological scoring demonstrated significantly accelerated tissue repair in the BC-MXene group compared with the bacterial cellulose and control groups ($p < 0.05$). Reduced inflammatory infiltration and increased granulation tissue maturity were observed as early as day 7, while epithelialization reached near-complete levels by day 14. These morphological improvements strongly correlated with the immunological and microbiological indicators included in the machine learning model (Table 4).

Statistical significance was set at $p < 0.05$. Ensemble models demonstrated the highest predictive performance, indicating their suitability for integrating complex biological datasets and forecasting treatment effectiveness.

To strengthen methodological validity in the context of a relatively small dataset ($n = 60$), repeated stratified cross-validation (5×10-fold) was implemented to ensure robust internal validation and minimize the risk of overfitting. For each machine learning algorithm, mean performance values were calculated together with 95% confidence intervals to provide statistical reliability of the predictive estimates. Among the evaluated models, gradient boosting demonstrated the highest and most stable

performance, achieving an AUC of 0.96 (95% CI: 0.91-0.99), while the random forest model yielded an AUC of 0.94 (95% CI: 0.88-0.97). Logistic regression showed comparatively lower predictive capacity with an AUC of 0.86 (95% CI: 0.79-0.92), indicating that ensemble-based algorithms are better suited for integrating multidimensional biological data derived from microbiological, immunological, and morphological assessments (Table 5).

To further justify the added value of artificial intelligence modeling, a baseline predictive approach based solely on early bacterial load reduction (CFU dynamics) was evaluated. This simplified model achieved an overall accuracy of 71.3% and an AUC of 0.74, which was substantially lower than the performance observed for the supervised machine learning algorithms, all of which exceeded 90% accuracy. This comparison confirms that multidimensional feature integration significantly enhances predictive performance compared to single-parameter statistical evaluation.

In addition to accuracy, sensitivity, and AUC, supplementary robustness metrics were calculated to provide a more comprehensive assessment of model reliability. The gradient boosting model achieved an F1-score of 0.91 and a specificity of 90.4%, demonstrating balanced classification performance between positive and negative treatment outcomes. Calibration analysis revealed a calibration slope of 0.97, indicating strong agreement between predicted probabilities and observed experimental outcomes, thereby supporting the clinical interpretability of the model.

Feature-importance analysis demonstrated that early bacterial clearance between days 3 and 7 was the strongest predictor of favorable therapeutic outcome. Cytokine normalization, particularly reductions in IL-6 and TNF-α levels, represented the second most influential predictive factor. Increased phagocytic activity contributed independently to outcome prediction, while morphological indicators such as accelerated granulation tissue formation and early epithelialization significantly improved model discrimination. SHAP-based interpretability analysis further confirmed that the integration of microbiological, immunological, and tissue-repair variables collectively strengthened predictive accuracy.

Assessment of overfitting showed minimal discrepancy between training and validation performance ($\Delta AUC < 0.03$), suggesting adequate generalization capability of the models. Learning-curve analysis indicated progressive stabilization of performance with increasing data exposure, supporting the internal consistency of the predictive framework despite the limited sample size.

Overall, the application of supervised machine learning algorithms demonstrated high predictive accuracy, robustness, and calibration in forecasting the antibacterial and immunological effectiveness of BC-MXene biocomposites. The multidimensional AI-based approach substantially outperformed conventional single-parameter statistical models and provided an integrated analytical framework for objective evaluation of advanced biomaterial performance in experimental purulent infection.

6 DISCUSSION

The results demonstrate that BC-MXene biocomposites provide superior antibacterial and immunological outcomes in experimental purulent infection models, and that these outcomes can be reliably predicted using artificial intelligence algorithms. The integration of AI allowed identification of key biological predictors, such as early bacterial load reduction and cytokine normalization, which traditional analyses might underestimate. From a medical perspective, AI-assisted prediction enhances precision in evaluating biomaterial effectiveness and supports personalized treatment strategies. Economically, predictive modeling can reduce unnecessary interventions, shorten treatment duration, and optimize resource utilization. Socially, improved healing outcomes contribute to reduced disability, faster return to normal activity, and improved patient quality of life. Overall, the combined use of BC-MXene biomaterials and AI-based analytics represents a forward-looking approach aligned with modern precision medicine and digital health paradigms.

7 CONCLUSIONS

This study demonstrated that BC-MXene biocomposites are a promising multifunctional platform for the local treatment of acute purulent infections. Compared with bacterial cellulose alone and conventional local therapy, the BC-MXene group showed a more pronounced reduction in bacterial load, faster normalization of inflammatory and immunological parameters, and better morphological indicators of tissue repair. These findings confirm that incorporation of MXene into the bacterial cellulose matrix significantly enhances the

antibacterial, immunomodulatory, and reparative performance of the biomaterial in infected wound environments.

A key contribution of this work is the demonstration that the therapeutic effectiveness of advanced wound biomaterials can be predicted with high reliability using artificial intelligence methods. The developed supervised machine learning models successfully integrated microbiological, immunological, hematological, and morphological variables into a unified predictive framework, with gradient boosting providing the best overall performance. This indicates that ensemble-based AI models are particularly effective for capturing complex nonlinear relationships in experimental biomedical data and for forecasting treatment outcomes in multifactorial infectious conditions.

The results also showed that early bacterial clearance, reduction of pro-inflammatory cytokines, restoration of phagocytic activity, and improved tissue-repair indicators were the most informative predictors of favorable outcome. This confirms that the biological effect of BC-MXene biocomposites should be interpreted as an integrated multidimensional response rather than as an isolated antibacterial effect. In this regard, the combination of biomaterial research with AI-driven analytics improves the objectivity, reproducibility, and translational relevance of preclinical evaluation.

From a practical perspective, the proposed biomaterial-AI framework may support more accurate assessment of advanced wound dressings, facilitate earlier identification of effective treatment strategies, and strengthen the transition from experimental studies to clinically applicable solutions. Although the present findings are limited by the animal model, relatively small sample size, and lack of external validation, they provide a strong foundation for future large-scale studies, independent model validation, and дальнейшую интеграцию molecular biomarkers, imaging features, and adaptive machine learning approaches. Overall, the study confirms that BC-MXene biocomposites and artificial intelligence can jointly form an effective basis for the development of intelligent, data-driven, and clinically translatable technologies for purulent wound management.

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