

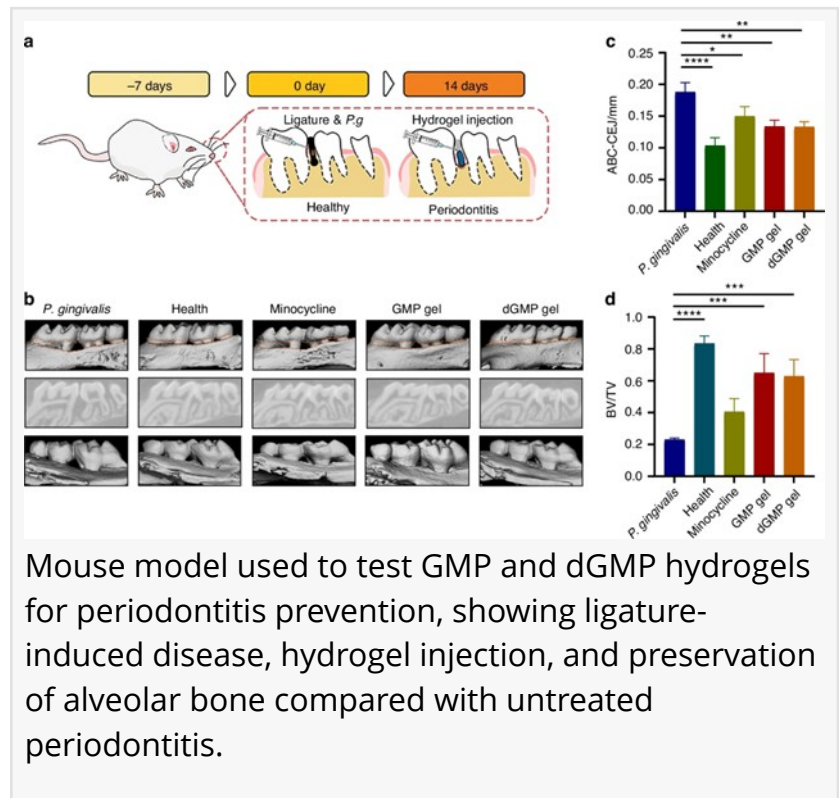
AI-Powered Screening Identifies Promising Hydrogels for Periodontal Therapy

New machine learning framework predicts promising nucleoside hydrogels before they are synthesized and tested in the lab

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/EINPresswire.com/ -- Artificial

intelligence is beginning to transform not only drug discovery but also the design of advanced biomaterials. In a new study, researchers combined machine learning with laboratory validation to develop a data-driven strategy for identifying bioactive nucleoside hydrogels for periodontitis treatment. By integrating predictive modeling with innovative molecular scoring methods, the work aims to streamline biomaterial discovery and accelerate the development of targeted therapies for oral health applications.



Periodontitis is one of the most common chronic inflammatory diseases worldwide and a leading cause of tooth loss in adults. Triggered by harmful bacteria that damage the gums and supporting bone, the disease often requires therapies that can simultaneously eliminate infection, reduce inflammation, and promote tissue repair. While biomaterials such as hydrogels have emerged as promising platforms for localized treatment, discovering formulations that combine potent antibacterial activity with safety and biocompatibility has traditionally depended on trial-and-error experimentation, which is slow, costly, and labor-intensive.

Seeking a faster and more systematic solution, researchers from Sichuan University—led by Prof. Hao Xu and Prof. Hang Zhao—developed a machine learning-guided strategy to identify bioactive nucleoside hydrogels for periodontal therapy. Corresponding author, Prof. Xu shares, “By integrating artificial intelligence-based predictive models with newly developed molecular scoring methods and experimental validation, we aimed to computationally screen thousands of

candidate molecules and focus laboratory testing on only the most promising ones.” The study was published in Volume 18 of [International Journal of Oral Science](#) on May 11, 2026.

To achieve this, the researchers combined computational screening with laboratory validation. They first compiled nine large bioactivity datasets from public databases and trained machine learning models to predict properties such as antibacterial activity, toxicity, antiviral potential, and anti-inflammatory effects based on thousands of molecular descriptors. They also introduced two novel evaluation metrics: the Molecular Bioactivity Specificity Index (MBSI), which identifies the dominant biological characteristic of a molecule, and the Composite Molecular Attribute Score (CMAS), which combines multiple desirable features including gelation potential, antibacterial activity, and biocompatibility into a single ranking system. After screening thousands of candidates, the highest-ranking molecules were synthesized and tested experimentally for hydrogel formation, mechanical properties, antibacterial activity against *Porphyromonas gingivalis*, biocompatibility, and efficacy in mouse models of periodontitis.

This AI-guided workflow ultimately identified two standout candidates: guanosine monophosphate (GMP) and deoxyguanosine monophosphate (dGMP). “Both candidates successfully formed stable supramolecular hydrogels with favorable mechanical properties such as self-healing and shear-thinning behavior” shares Prof. Zhao. He adds, “In laboratory experiments, the hydrogels effectively inhibited *Porphyromonas gingivalis* while exhibiting excellent biocompatibility and minimal toxicity.” In mouse models of periodontitis, treatment reduced bacterial burden and inflammation, preserved alveolar bone, and promoted tissue repair, demonstrating efficacy comparable to that of the antibiotic minocycline. When administered early, the hydrogels also helped prevent disease progression.

Beyond identifying two promising therapeutic materials, the study highlights how artificial intelligence can transform biomaterial discovery. Rather than relying primarily on empirical testing, researchers can use predictive models to rapidly narrow vast chemical spaces and prioritize candidates with the highest likelihood of success. The introduction of MBSI and CMAS further strengthens this approach by enabling multiple performance characteristics to be evaluated simultaneously, offering a practical framework for balancing efficacy, safety, and functionality during material design. Together, these advances could shorten development timelines, reduce research costs, and improve the efficiency of creating clinically relevant biomaterials.

The implications extend well beyond periodontitis. The same computational framework could be adapted to develop hydrogels for drug delivery, wound healing, tissue engineering, regenerative medicine, and other oral health applications. As larger datasets become available and more sophisticated artificial intelligence methods are incorporated, the approach may enable increasingly accurate predictions and even support the design of personalized biomaterials tailored to specific therapeutic needs.

Overall, this study demonstrates the power of combining machine learning with experimental

validation to accelerate the rational design of multifunctional biomaterials. By successfully identifying and validating GMP- and dGMP-based hydrogels for periodontal therapy, the researchers provide a proof of concept for a data-driven strategy that could reshape how next-generation therapeutic hydrogels are discovered and developed across a wide range of biomedical fields.

Reference

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About Sichuan University

Sichuan University is a research university located in Chengdu, China, and widely recognized as one of the country's leading higher education institutions. It was formed through the merger of several historic universities, including the former West China University of Medical Sciences, giving it a strong foundation in medical and health sciences. The university offers a broad range of disciplines across medicine, engineering, natural sciences, humanities, and social sciences. Its West China medical campuses, particularly the West China Hospital of Stomatology, are internationally recognized for dental and biomedical research. Sichuan University is part of China's elite "Double First-Class" initiative.

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About Prof. Hang Zhao from Sichuan University

Prof. Hang Zhao is a researcher affiliated with Sichuan University, China, at the West China School of Stomatology. His research focuses on novel oral preparations and targeted delivery systems. He received national and ministerial youth talent grants in 2019 and 2018. He has published over 30 high-level papers in top journals, presided over more than 10 national research projects, and owns 30 patents (5 US patents). Five patents have been industrialized with 12.8 million RMB transformation revenue, and two related products are on sale. He has gained the Second Prize of Huaxia Medical Award and the First Prize of Sichuan Provincial Natural Science Award.

About Prof. Xu Hao from Sichuan University

Prof. Hao Xu is a researcher affiliated with Sichuan University, China, at the West China School of Stomatology. His research focuses on precise diagnosis and treatment of oral diseases based on multimodal data. He has published 33 papers as the first or corresponding author in journals including Nature Communications and Journal of Dental Research. He has been named an Elsevier Highly Cited Chinese Researcher and presided over 2 General Program projects supported by the National Natural Science Foundation of China.

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