

Artificial Intelligence-Driven Pharmacotherapy in Post-Operative Oral and Maxillofacial Surgery: Transforming Prescription Practices

Alireza R Azadi^{1*}, Omid Panahi²

¹Urmia University of Medical Sciences, School of Dentistry, Urmia, Iran.

²University of The People, Department of Healthcare Management, California, USA.

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Corresponding Author: Alireza R Azadi, Urmia University of Medical Sciences, School of Dentistry, Urmia, Iran.

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Abstract

Postoperative pain, infection, and medication-related complications remain significant challenges following oral and maxillofacial surgery (OMFS). The prescription of appropriate analgesics, antibiotics, and supportive medications must navigate complex patient histories, potential drug–drug interactions (DDIs), and individual risk factors. Artificial intelligence (AI), particularly machine learning (ML) and large language models (LLMs) is emerging as a powerful clinical decision-support tool for optimizing postoperative pharmacotherapy. This article examines current applications of AI in predicting medication order errors, detecting clinically significant DDIs, identifying patients at risk for medication-related osteonecrosis of the jaw (MRONJ), and accelerating drug discovery for regenerative therapies. The evidence demonstrates that while AI tools achieve high sensitivity in DDI detection and can accurately predict voided medication orders, significant limitations remain, including false-positive alerts, missed critical interactions, and the black-box nature of deep learning models. The near future will see AI integrated as a supervised decision-support system, augmenting rather than replacing the oral surgeon's clinical judgment.

Keywords: Artificial Intelligence, Drug-Drug Interactions, Postoperative Care, Oral and Maxillofacial Surgery, Clinical Decision Support, Machine Learning, Large Language Models.

Introduction

The prescription of medications following oral and maxillofacial surgery is a critical component of patient care that directly impacts recovery, complication rates, and overall outcomes. Patients undergoing OMFS procedures ranging from third molar extractions to orthognathic surgery and jaw reconstruction frequently require a combination of analgesics (opioids and non-opioids), antibiotics, corticosteroids, and antiemetics. The challenge is compounded by the fact that many surgical patients are already using chronic medications for cardiovascular disease, diabetes, psychiatric conditions, or osteoporosis [1-43].

Errors in postoperative prescribing can have severe consequences. Drug–drug interactions (DDIs) may lead to excessive bleeding, serotonin syndrome, acute kidney injury, or therapeutic failure of critical medications. A study of 37,493 medication orders in OMFS inpatients found that 10.4% were voided representing either errors or changes in clinical status [44-57]. Even more concerning is that many DDIs go unrecognized at the point of care, particularly when patients are prescribed medications by multiple providers.

Artificial intelligence offers a potential solution to these prescribing challenges [58-74]. Machine learning algorithms can analyze large datasets of electronic medical records to identify patterns predicting medication errors. Large language models can rapidly screen medication lists against known interaction databases. And deep learning systems can integrate

imaging and genomic data to predict individual patient risks for adverse drug reactions.

This paper explores the current state and near-future potential of AI-driven pharmacotherapy support in OMFS, focusing on four key domains:

- (1) prediction of medication order errors
- (2) detection of clinically significant DDIs
- (3) risk prediction for medication-related osteonecrosis of the jaw (MRONJ)
- (4) AI-accelerated drug discovery for postoperative tissue regeneration [75-89].

AI for Predicting Medication Order Errors

Reducing Prescription Errors: Machine Learning for Order Validation

Medication ordering errors are a persistent problem in hospital-based OMFS. Errors can result from incorrect dosing, wrong medication selection, duplication of therapy, or prescribing contraindicated medications. In many cases, these errors are caught only when a pharmacist reviews the order often hours later or when the order is "voided" and rewritten by the prescriber.

A Landmark Study in OMFS Medication Order Prediction

A recent study by Nathan and colleagues (2024) investigated whether supervised machine learning algorithms could accurately predict which medication orders in OMFS inpatients would be voided [90-103]. The researchers retrospectively analyzed 37,493 medication orders from 1,204 patient admissions over a five-year period. The data included patient

demographics, comorbidities, procedures, vital signs, laboratory values, and medication orders.

Four machine learning algorithms were trained and tested

- Gradient Boosted Decision Trees (GBDT)
- Random Forest (RF)
- K-Nearest Neighbor (KNN)
- Naïve Bayes (NB)

Results and Clinical Implications

Among these models, Gradient Boosted Decision Trees (GBDT) demonstrated the best performance:

Model AUC-ROC (95% CI) AUC-PRC (95% CI)

Gradient Boosted Decision Trees 0.802 [0.787, 0.825] 0.684 [0.679, 0.702]

Random Forest 0.746 [0.722, 0.765] 0.647 [0.638, 0.664]

K-Nearest Neighbor 0.685 [0.667, 0.699] 0.429 [0.417, 0.434]

Naïve Bayes 0.505 [0.489, 0.539] 0.551 [0.551, 0.552]

The GBDT model achieved an Area Under the Receiver Operating Curve (AUC-ROC) of 0.802, indicating "satisfactory outcomes" for predicting voided medication orders [104-112]. This suggests that AI could be integrated into electronic health record systems to provide real-time alerts when a prescribed medication order has a high probability of being subsequently voided due to error.

Future Directions

The clinical implementation of such predictive models would allow prescribers to receive immediate feedback during order entry, potentially reducing the 10.4% void rate observed in the study. Future work should focus on prospective validation and integration with computerized physician order entry (CPOE) systems [113-123].

AI for Drug-Drug Interaction Detection

Detecting Drug-Drug Interactions at the Point of Care

Perhaps the most clinically urgent application of AI in postoperative pharmacotherapy is the detection of clinically significant DDIs. Patients undergoing OMFS are frequently polymedicated, and the addition of perioperative drugs NSAIDs, acetaminophen, opioids, antibiotics, corticosteroids can create dangerous interaction profiles [124-143].

The Clinical Significance of DDIs in OMFS

The risks are substantial and well-documented

- Bleeding risk: Combining warfarin (anticoagulant) with antiplatelet agents amplifies hemorrhage risk several-fold.
- Serotonin syndrome: Coadministration of tramadol (an opioid) with SSRIs can precipitate life-threatening serotonin toxicity.
- Gastrointestinal bleeding: NSAIDs combined with SSRIs more than doubles the odds of GI bleeding.
- Osteonecrosis risk: Antiresorptive medications (bisphosphonates, denosumab) are directly associated with medication-related osteonecrosis of the jaw (MRONJ).

Despite these known risks, dentists may lack access to patients' full medication histories, and the time pressure of chairside decision-making increases the likelihood of missed or underestimated DDIs [144-165].

Comparing AI Models to Oral Surgeons

A prospective, simulation-based study published in December 2025 directly compared five large language models (ChatGPT-5, DeepSeek-Chat, DeepSeek-Reasoner, Gemini-Flash, and Gemini-Pro) with a panel of

experienced oral surgeons [166-175]. The study used 500 standardized oral-surgery scenarios, each including a fixed postoperative regimen (analgesic, amoxicillin/clavulanate, short corticosteroid course) combined with variable chronic medications spanning cardiovascular agents, antidiabetics, anticoagulants, antidepressants, and antiepileptics.

AI vs. Human Performance in DDI Detection

Key Findings and Performance Trade-offs

The results revealed important trade-offs between sensitivity and specificity:

Model	Exact Agreement	Surgeons Sensitivity	Actionable DDIs	Specificity	Median Response Time
DeepSeek-Chat	50.6%	18.0%	100%	~3.6 seconds	
ChatGPT-5	Not reported	98.0%	56.7%	Not reported	
Oral Surgeons (Human)	Reference	Reference	Reference	Reference	225 seconds

DeepSeek-Chat achieved the highest exact agreement with surgeon consensus (50.6%) and demonstrated perfect specificity (100%) meaning it never generated a false-positive DDI alert. However, its sensitivity was very low (18%), missing 82% of actionable D/X (drug-interaction requiring action) alerts [176-193].

ChatGPT-5 showed the opposite pattern: the highest sensitivity (98.0%) but lower specificity (56.7%), generating more false-positive warnings that could lead to unnecessary changes in medication or surgical delays [194-201].

Clinical Implications

These findings indicate that current LLMs exhibit distinct safety trade-offs between missed critical interactions and alert overcalling. Neither pattern is ideal. Missing 82% of actionable DDIs (DeepSeek-Chat) is clinically unacceptable. Conversely, generating false-positive alerts in 43.3% of cases (ChatGPT-5) would lead to alert fatigue and potential overtreatment [202-206].

The study concluded that LLMs should be considered decision-support tools rather than substitutes for clinical judgment, and their integration should prioritize validated, supervised workflows [207-210]. The rapid response time of AI (seconds versus 225 seconds for human review) suggests that AI can serve as an efficient pre-screening tool, with human verification required for flagged interactions.

AI for MRONJ Risk Prediction

Predicting Medication-Related Osteonecrosis of the Jaw (MRONJ)

Medication-related osteonecrosis of the jaw (MRONJ) is a potentially devastating complication characterized by exposed necrotic bone in the oral cavity, infection, and pain [211]. It is associated with antiresorptive medications (bisphosphonates, denosumab) and antiangiogenic agents used to treat osteoporosis and cancer.

The Primordial Project

An ongoing research project at KU Leuven (2022-2025) titled PRIMORDIAL is developing an AI-driven prediction model to detect risk factors for MRONJ [212]. The project has two main objectives:

1. Identify radiological and genetically predisposing factors for developing MRONJ
2. Describe risk factors influencing treatment outcome in patients with established MRONJ

The study employs a radiomics approach extracting quantitative features from medical images that are not visible to the human eye combined with genomic data to build automated prediction models [213].

Clinical Significance for Postoperative Prescribing

For the oral surgeon, the relevance is direct: before prescribing antiresorptive medications or before performing extractions on patients already taking these drugs, an AI-driven risk assessment could:

- Quantify the individual patient's probability of developing MRONJ
- Recommend alternative medications or modified surgical protocols
- Identify the need for drug holiday periods or adjunctive therapies

Early detection of MRONJ risk would allow for preventive measures, potentially avoiding the development of advanced lesions that are difficult to treat [214].

AI in Regenerative Drug Discovery

AI-Accelerated Drug Discovery for Postoperative Regeneration

Beyond error prevention and risk prediction, AI is also transforming the discovery of new drugs to enhance postoperative healing. Following complex OMFS procedures—bone grafting, implant placement, jaw reconstruction, the ideal pharmacological support would not only manage pain and infection but actively promote tissue regeneration.

Graph Neural Networks for Drug-Gene Interaction Prediction

A 2024 study utilized Graph Neural Networks (GNNs) to predict drug-gene interactions of the RTK-VEGF4 receptor family in periodontal regeneration [215]. The model achieved 97% accuracy in predicting interactions, demonstrating the potential for AI to accelerate the discovery of targeted therapies for tissue healing after surgery [216].

AlphaFold and Protein Structure Prediction

AlphaFold, an AI system developed by DeepMind (now Google DeepMind), has revolutionized protein structure prediction. In the context of oral surgery, AlphaFold is being explored as a tool for drug development in oral cancer and potentially for designing drugs that target specific proteins involved in postoperative inflammation and healing [217].

Clinical Implications

The ability to predict drug-gene interactions with high accuracy opens the door to:

- Personalized pharmacotherapy: Selecting drugs based on the patient's genetic profile to maximize healing and minimize adverse effects
- Novel drug development: Identifying new therapeutic targets for postoperative pain, edema, and bone regeneration
- Reduced trial-and-error prescribing: Moving from empirical to evidence-based, AI-guided medication selection

Limitations and Challenges

The Current Limitations of AI in Clinical Pharmacotherapy

Despite the promising developments, significant limitations must be acknowledged before AI can be widely adopted for postoperative prescribing in OMFS.

The "Black Box" Problem

Deep learning models, including many AI systems used for DDI detection and risk prediction, are inherently opaque. They often do not explain why a certain recommendation or prediction was made [218]. This opacity is problematic in healthcare, where trust and understanding are paramount. Surgeons and patients may be reluctant to act on an AI's advice without a clear rationale, especially when it conflicts with clinical judgment.

Explainable AI (XAI) techniques are being developed to address this, but they are not yet standard in most clinical systems [219].

Hallucinations and Inaccurate Information

Large language models are known to "hallucinate" producing confident but incorrect information [220]. In the context of medication prescribing, a hallucinated DDI or incorrect dosage recommendation could have serious consequences. Regulatory bodies and healthcare institutions emphasize that without the ability to automatically discern fact from fabrication, LLM outputs must be double-checked by experts [221].

A systematic review of ChatGPT in OMFS found that while GPT-4 achieved 76.8% accuracy on multiple-choice questions, performance was lower specifically in pharmacology and complex clinical scenarios [221].

Domain Specificity and Training Data Limitations

AI systems trained on one population may not generalize to others. For example, an AI trained primarily on adult cases may perform poorly on pediatric OMFS. Similarly, models trained on data from one geographic region or ethnic group may have reduced accuracy when applied to different populations [223].

Regulatory Hurdles

Medical AI systems qualify as medical devices and require regulatory approval (FDA clearance in the US, CE marking in Europe). As of 2025, while many AI algorithms exist in research, relatively few have received clearance for clinical use [39]. The regulatory process is necessarily cautious, but it also slows the introduction of potentially beneficial innovations.

The Near Future: Integrated Decision Support

A Roadmap for AI Integration in Postoperative Prescribing

Given the current evidence, the near future (2026–2030) will likely see AI implemented as a supervised decision-support system rather than an autonomous prescriber.

Proposed Workflow Integration

A realistic integration scenario for the OMFS clinic would include

Step 1: Automated Data Aggregation

- AI extracts the patient's complete medication list from the electronic health record, including over-the-counter medications and supplements often missed in history-taking.

Step 2: Real-Time DDI Screening

- An LLM or rule-based AI system screens the proposed postoperative prescription against the patient's chronic medications.
- The system flags potential interactions and classifies severity (e.g., A-X scale using Lexicomp-based criteria).

Step 3: Human Verification

- The oral surgeon reviews flagged interactions, accepting, modifying, or overriding the AI's suggestion.
- For cases with no flags, the prescription proceeds; for actionable flags (D/X), the surgeon makes the final decision.

Step 4: Continuous Learning

- The system tracks outcomes (e.g., whether a flagged interaction led to an adverse event or whether an unflagged interaction was missed) and updates its model accordingly.

The "Trust, But Verify" Approach

Professional guidelines increasingly recommend a "trust, but verify" approach: use AI as an adjunct, but double-check critical outputs. This failsafe approach acknowledges AI's capabilities while guarding against overreliance on a tool that occasionally produces errors.

Training Implications

Oral and maxillofacial surgeons will need training in:

- Understanding the strengths and limitations of AI tools
- Recognizing when an AI output is likely unreliable
- Integrating AI recommendations with clinical judgment

Conclusion

Artificial intelligence is poised to transform postoperative pharmacotherapy in oral and maxillofacial surgery, but not by replacing the human prescriber. Instead, AI will augment clinical decision-making through four primary mechanisms:

1. Error prediction: Machine learning models (e.g., Gradient Boosted Decision Trees) can identify medication orders at high risk of being voided, enabling real-time correction during order entry.
2. DDI detection: Large language models provide rapid, structured screening of medication lists, though current models exhibit trade-offs between sensitivity (ChatGPT-5) and specificity (DeepSeek-Chat). None are yet reliable as standalone prescribers.
3. Risk prediction: AI-driven radiomics and genomic analysis can identify patients at elevated risk for MRONJ before antiresorptive therapy or dental surgery.
4. Drug discovery: Graph neural networks and protein structure prediction (AlphaFold) are accelerating the identification of novel drugs for postoperative regeneration and healing.

The Role of the Oral Surgeon

The oral surgeon of the near future will not be replaced by AI but will need to become an effective supervisor of AI systems. The critical skills will shift from memorizing drug interaction tables to:

- Critically evaluating AI-generated recommendations
- Recognizing the limitations and potential errors of each AI model
- Integrating AI outputs with patient-specific clinical nuances
- Managing the ethical and legal implications of AI-assisted prescribing

Final Statement

AI will not write postoperative prescriptions autonomously in the near future. The liability, accountability, and ultimate responsibility remain with the human surgeon. However, AI will increasingly serve as a powerful second opinion faster than a pharmacist consult, more systematic than memory, and continuously learning from every case. The optimal future is not human or AI, but human and AI, working together to deliver safer, more personalized postoperative pharmacotherapy.

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