ChemEngineering

Article

Industry 5.0 and Digital Twins in the Chemical Industry: An Approach to the Golden Batch Concept

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Abstract

In the context of industrial digitalization, the Industry 5.0 paradigm introduces digital twins as a cutting-edge solution. This study explores the concept of digital twins and their integration with the Industrial Internet of Things (IIoT), offering insights into how these technologies bring intelligence to industrial settings to drive both process optimization and sustainability. Industrial digitalization connects products and processes, boosting the productivity and efficiency of people, facilities, and equipment. These advancements are expected to yield broad economic and environmental benefits. As connected systems continuously generate data, this information becomes a vital asset, but also introduces new challenges for industrial operations. The work presented in this article aims to demonstrate the possibility of generating advanced tools for process optimization. This, which ultimately impacts the environment and empowers people in the processes, is achieved through data integration and the development of a digital twin using open tools such as NodeRed v4.0.9 and Python 3.13.5 frameworks, among others. The article begins with a conceptual analysis of IIoT and digital twin integration and then presents a case study to demonstrate how these technologies support the principles of the Industry 5.0 framework. Specifically, it examines the requirements for applying the golden batch concept within a biological production environment. The goal is to illustrate how digital twins can facilitate the achievement of quality standards while fostering a more sustainable production process. The results from the case study show that biomaterial concentration was optimized by approximately 10%, reducing excess in an initially overdesigned process. In doing so, this paper highlights the potential of digital twins as key enablers of Industry 5.0—enhancing sustainability, empowering operators, and building resilience throughout the value chain.

Keywords: Industry 5.0; Digital Twin (DT); Industrial Internet of Things (IIoT); golden batch; chemical industries; industrial process optimization

Academic Editors: Vincenzo Russo and Roumiana Petrova Stateva

Received: 19 February 2025
Revised: 13 June 2025
Accepted: 16 July 2025
Published: 25 July 2025

Citation: Redchuk, A.; Walas Mateo, F. Industry 5.0 and Digital Twins in the Chemical Industry: An Approach to the Golden Batch Concept. *ChemEngineering* **2025**, *9*, 78. https://doi.org/10.3390/chemengineering9040078

1. Introduction

Building on the insights from the doctoral thesis referenced in [1], and research on digital twins (DTs) in the process industry [2], this work proposes moving beyond the conventional IIoT paradigm by addressing new architectural strategies for data integration and the gradual incorporation of artificial intelligence (AI) into industrial environments. DTs emerge as a key area of interest, with the potential to improve the complexity and accuracy of data models while enabling the optimization of industrial operations [3].

In this scenario, both academic and industrial sectors show increasing interest in exploring digital twins, particularly their integration with IIoT systems and their application in prescriptive analytics aimed at process optimization. DTs provide a structured approach to unify data from operational activities and deliver analytical tools to support process analysis and enhancement. This research is grounded in the ISA-95 standard [4] and the RAMI 4.0 framework (Reference Architecture Model Industrie 4.0), developed by the German Electrical and Electronic Manufacturers' Association (ZVEI) [5]. DT technology has surged as a powerful and innovative alternative to conventional system management methods such as virtualization and containerization. While those traditional approaches mainly concentrate on abstracting software environments and enhancing deployment flexibility, DTs provide a comprehensive and dynamic representation of physical systems by virtually replicating their real-world behavior. This capability allows for real-time monitoring, simulation, and optimization of industrial processes. A key strength of DTs lies in their ability to enable secure and seamless integration between Operational Technology (OT) and Information Technology (IT) systems. Such integration is essential for the large-scale implementation of Industrial Internet of Things (IIoT) solutions and for extending OT functions into cloud-based platforms. As a result, DTs pave the way for smarter, more scalable, and adaptive manufacturing systems.

The study cited in [6] highlights that modern smart manufacturing is evolving into a sophisticated network of interconnected systems. These systems are increasingly capable of linking raw materials, production lines, logistics networks, and maintenance activities into a cohesive framework, thanks to the adoption of IIoT technologies. This connectivity gives rise to cyber-physical production systems (CPPSs), which blend the digital and physical aspects of manufacturing operations throughout the entire product lifecycle. The development of these CPPSs is being driven by advances in digital manufacturing (DM) technologies, which now support not only product design but also factory layout optimization, system reengineering, and in-depth process evaluation. These capabilities allow manufacturers to streamline operations, minimize waste, and quickly adapt to market shifts—all within a virtual and data-centric environment.

Nonetheless, it is crucial to broaden this perspective by considering the emerging Industry 5.0 (I5.0) paradigm. In contrast to Industry 4.0, which emphasized automation and digitization, Industry 5.0 places a stronger focus on human-centered innovation, sustainability, and resilience. The I5.0 approach promotes (1) empowering human operators in decision-making roles, (2) fostering environmentally responsible industrial practices, and (3) building more flexible and robust value chains that can withstand disruptions. Although IIoT technologies have played a major role in advancing manufacturing digitalization, they fall short in fully addressing the wider objectives of Industry 5.0—especially in terms of people empowerment and operational transparency [7].

This is where DTs become particularly relevant. As highlighted in [8], DTs are essential tools for achieving the production and sustainability goals envisioned in Industry 5.0. Their ability to collect, process, and analyze vast amounts of data throughout the production cycle makes them invaluable for real-time optimization and strategic planning. One of the most notable advantages of DTs over conventional data-driven tools, such as machine learning (ML), lies in their interpretability. While ML models often operate as "black boxes", producing outputs without clear insights into internal logic or causality, digital twins function more like "glass boxes". They provide visibility into system behavior and process dynamics, allowing engineers and operators to understand not just what is happening, but why it is happening. This transparency is critical for empowering human decision-makers, fostering trust in technology, and enabling collaborative human–machine environments—one of the cornerstones of Industry 5.0. The case developed in this article considers that high-fidelity dynamic models of bioreactors are rarely applied in industrial settings, despite their potential. McMillan et al. [9] affirm that their use has remained largely confined to academia due to several practical challenges. One of the most significant barriers is the difficulty in accurately defining the kinetic parameters required for the models to reliably replicate the behavior observed at different scales—ranging from laboratory experiments to pilot plants and full-scale production facilities. This complexity is compounded by the intricate and often variable nature of biological pathways, making model calibration and validation a demanding task in real-world applications.

Some Preliminary Findings

An initial bibliographic research was carried out to identify and understand the key issues addressed in this study. To lay the groundwork for the research, a selection of pertinent scholarly articles was examined, providing valuable perspectives that supported the development of the case analysis. The relationship between the Industrial Internet of Things (IIoT) and digital twins (DTs) is explored from various perspectives in multiple publications [10–16]. These sources offer important insights that inform the bibliometric research on the application of DT in process industries. To begin with the review, Yuchen et al. [10] highlight that IIoT, DTs, and advancements in mobile networks are currently driving the development of decentralized, self-managed cyber-physical production systems (CPPSs) in industry. DTs enable mobile networks to deliver adaptive and dynamic configurations for cooperative CPPSs. Furthermore, the authors propose that trustworthy cooperation can be achieved using blockchain technology. They present a solution where blockchain is used to cross-verify and validate newly added blocks with the assistance of validator nodes. The study by Aloqaily et al. [11] proposes a product quality control approach based on a semantic DT information model for terminal devices. This model allows for flexible parameter configuration and adjustment of the devices to meet the requirements of flexible production and manufacturing. The authors argue that their approach improves hardware resource utilization and enhances the efficiency of product quality assessments, while also reducing deployment costs. Additionally, the system offers adaptability to different product types and industrial environments. according to [12], DT technology addresses the requirements of IIoT by enabling system simulation, monitoring, and optimization. The paper examines the integration of the formal modeling method, Petri nets, within the context of Networked Digital Twins (NDTs) for modeling IIoT. The authors introduce a data-driven Petri net approach and demonstrate its effectiveness in executing what-if scenarios based on network parameters, enabling predictions of the Packet Delivery Ratio and real-time fault detection. In [13], the authors present an implementation of a digital twin that connects through the IIoT architecture using Node Red. This paper provides insightful information to replicate the architecture in the case to be addressed. Furthermore, to support the conceptual framework of this research, the work by [14] is cited. The authors argue that DTs are promising tools for replicating and analyzing production systems in real time. A DT should be capable of offering well-defined services to support activities such as monitoring, maintenance, management, optimization, and safety. This paper focuses on the integration level of the DT with the control systems of the physical plant, particularly with Manufacturing Execution Systems (MESs), within the context of the ISA-95 automation pyramid. It also compares the services offered by the proposed DT with those in reference models.

The paper [15] provides a concrete example of cybersecurity risk mitigation strategies, considering the vulnerabilities that arise in DT/IIoT integration. The study presents a thorough security evaluation aimed at identifying and mitigating potential integration weaknesses. It highlights that the implementation of security features on devices also influences overall performance. The research seeks to balance robust security with smooth operational efficiency. Ultimately, it aims to make a valuable contribution to enhancing Internet of Medical Things (IoMT) security, supporting the deployment of secure healthcare technologies, and fostering public trust.

In their article, Li et al. [16] make an interesting contribution focused on the research of green performance evaluation methods of smart manufacturing to promote the transformation of the manufacturing industry to green smart manufacturing from the perspective of performance evaluation. The authors affirm that green smart manufacturing represents the strategic direction for the sustainable development of the manufacturing industry. It aims to achieve a balanced integration of environmental, social, and economic performance within manufacturing systems—ultimately promoting sustainable consumption and production. Accomplishing this goal requires the support of appropriate technologies and policies.

Therefore, this paper begins by proposing a conceptual framework about DTs and experience in the process industry. Then, the case using a DT to ease achieving a golden batch in a seed inoculant firm, a biological process, is presented. In this paper, a golden batch is linked to a biological process, which refers to the ideal production cycle that serves as a standard for optimal quality, consistency, and efficiency. It represents the batch that successfully meets all critical quality parameters and process performance goals, such as optimal biomaterial concentration, yield, pH levels, and temperature control, with minimal variation.

2. Conceptual Framework

The concept of the digital twin (DT) was first introduced by Grieves in 2003 [17]. A widely accepted definition comes from Stark [18], who describes a digital twin as “the digital representation of a unique asset (such as a product, machine, service, or product-service system) that mirrors its characteristics, state, and behavior using models, data, and information”. According to Stark, a DT is composed of three key components: the Digital Model (also known as the Digital Master Model), the Digital Shadow (real-world data captured from the asset), and the integration of both elements.

Stravoulakis et al. [19] classify digital twins into five categories based on their level of abstraction and complexity in data analysis. For the purposes of this study, the focus is on the first type, which combines 2D or 3D graphical representations of physical assets with operational data obtained through sensors. This type supports descriptive analytics that help analyze how a piece of equipment or process behaves. It enables statistical assessments, identification of failure modes, and evaluation of key performance indicators (KPIs) to make visible operation status.

McMillan et al. [20] outline the steps for developing a DT of the first type, which is the focus of our in-depth study. The authors describe three phases: model development, DT creation, and adjustment/configuration. The first phase involves reproducing the virtual structure that mirrors the physical element (equipment or process) under study. The second phase integrates the data that animate the virtual model. The third phase entails configuring parameters and software essential for its operation, including settings for elements that will act as sensors or actuators within the model, such as speeds, sensor ranges, and other characteristics.

According to findings in previous studies [21], the importance of robust IIoT infrastructure for integration must be emphasized, specifically, transferring data from the plant floor to the model. In this context, cybersecurity issues are critical to ensure the DT operates reliably, making the accessibility of operational data through the OPC UA communication protocol highly significant.

Data collection and its integration have been addressed by the International Society for Automation (ISA) [4] and the International Electro-technical Commission (IEC) [22]. For example, the IEC 62264 multilayer standard based on the ISA-95 specifications [4] defines a framework for exchanging information models that allows the integration of applications that run in areas of management and operations. Companies that comply with this standard can define interfaces between control and management functions, allowing them to make informed decisions about the data to exchange so that costs and risks are kept low in the event of implementation errors.

Another reference standard to consider for this article is the European Reference Architectural Model Industry 4.0 (RAMI 4.0) [5], which advocates a close coordination of IT and OT. To achieve this, RAMI 4.0 offers a high-level reference architecture designed to cover the diverse range of Industry 4.0 scenarios. The communication layer integrates the concept of Industry 5.0 into the OPC UA standard, positioning this item as the sole solution that ensures interoperability within the OT layer [22].

At this point, an issue to observe is how to address privacy concerns in IIoT/DT ecosystems. This is not a trivial aspect; the article from Salam et al. [23] addresses potential ethical/safety issues in the process of sharing data across stakeholders. Industries are currently applying artificial intelligence and machine learning to improve efficiency, employee safety, and enhance product quality. In manufacturing companies, ongoing maintenance of production lines and machinery results in significant expenses, which also have a major impact on the bottom line of any asset-dependent production operation [24].

According to Martínez-Plumed et al. [25], ML, or machine learning, is the area of artificial intelligence that deals with developing algorithms (and programs) capable of learning and constitutes, along with statistics, the heart of intelligent data analysis. The principles followed in machine learning are like those applied in data mining: the machine learns a model from examples and uses it to solve the problem.

One of these models is the autoencoder [26]. The autoencoder is an unsupervised learning model that identifies patterns in a dataset. Its basic structure consists of two parts: an encoder, which takes the input data and transforms it into a lower-dimensional representation, and a decoder, which uses this compressed representation to reconstruct the original data as faithfully as possible. The article from Salam et al. [27] provides a methodological reference for autoencoder applications in industrial processes. In this article the authors study the balance between privacy preservation and learning efficiency within the context of the Secure Collaborative Learning Algorithm (SCLA).

A Case Study to Reach a Golden Batch Using Analytics

This case study highlights the need to optimize and analyze the data in the production batches of a seed inoculant plant. First of all, a challenge was detected: the need to standardize the quality levels of the batches. Looking to improve the processes, the firm realized the importance of continuous monitoring that enables the identification of how close we are to the "golden batch", that is, the ideal batch that meets all established quality standards. The process under study required several teams to upload information about the biological process to a computer. The purpose is to automate this flow of information, so that the data, when uploaded from the production equipment, is automatically transferred to an analytical platform that can effectively evaluate the quality level of each batch. This would not only help standardize quality levels but would also ease the identification of opportunities for improvement and optimization in real time.

Achieving a “golden batch” in the production of biological inoculants for agriculture involves ensuring the consistency, quality, and effectiveness of the product in each batch. Since this is a biological process, it is essential to monitor and control several parameters at different stages of the process, which is influenced by many factors, with quite a few of them interacting with each other. It is fair to say that the process is immensely complex. Parameters to be controlled can be grouped into raw material, microbial strain, culture parameters, microbiological control, and characterization of the final product.

The plant is a relatively small one with seven assets. Each asset has about 15 variables to sense. They are parameters like pH, temperature, and dissolved oxygen sensors; chromatography to evaluate secondary metabolites; automated cell counters (e.g., flow cytometry); and rapid viability tests (e.g., colorimetry or specific stains). Controlling these parameters will reduce variations between batches and ensure a reliable and effective product for use in agriculture.

The plant has mature OT infrastructure, but information is not completely integrated, and there is a need to eliminate some silos. Then, to have the data available for integration and analysis, it was decided to advance in the adoption of an IIoT architecture. For this purpose, a Gateway-type device was incorporated to take the data of the plant operation, which is found in the OT network, to the cloud. For the integration of the information of the processes, the OPC UA server that incorporates the existing SCADA platform in the company is used and enables the interoperability of the data so that it can finally be viewed on the IIoT platform. Then, data from the production process, such as process parameters (temperature, pH, humidity, oxygen, etc.), composition of the culture medium, process times and stages, and final product quality results, is stored in a MongoDB database.

The data was organized and analyzed using High-Performance Numerical Operations (NumPy). Figure 1 shows the analysis of IIoT sensor data using NumPy. The blue line with markers represents the sensor readings over time, while the red dashed line indicates the mean temperature. The shaded red region represents the standard deviation range, helping to visualize normal variations in temperature. This approach allows quick identification of anomalies—any reading significantly outside the shaded region could indicate a potential issue in the system.

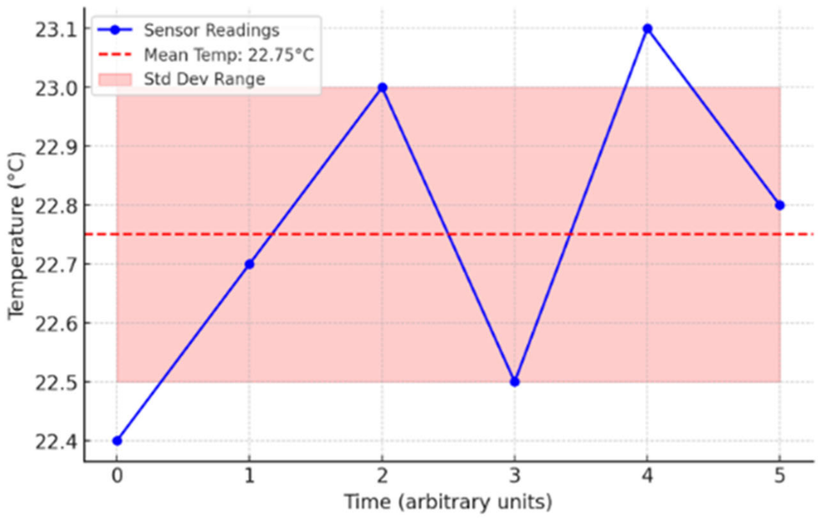

Figure 1. IIoT sensor data analysis using NumPY.

As shown in Figure 1, IIoT sensor data analysis using NumPY and the Matplotlib 3.10.0 and Seaborn 0.13 libraries was conducted to analyze data by generating graphs showing important information in a more understandable way. Figure 2 shows a correlation graphic using Matplotlib and Seaborn libraries to analyze the impact of the most critical variables in the production processes of agricultural seed inoculants. The values in the correlation matrix indicate the strength and direction of the correlation between the variables. A value close to 1 indicates a strong positive correlation, while values close to −1 indicate a negative correlation. This helps to identify which parameters most influence biomass production and the biological activity of the inoculant.

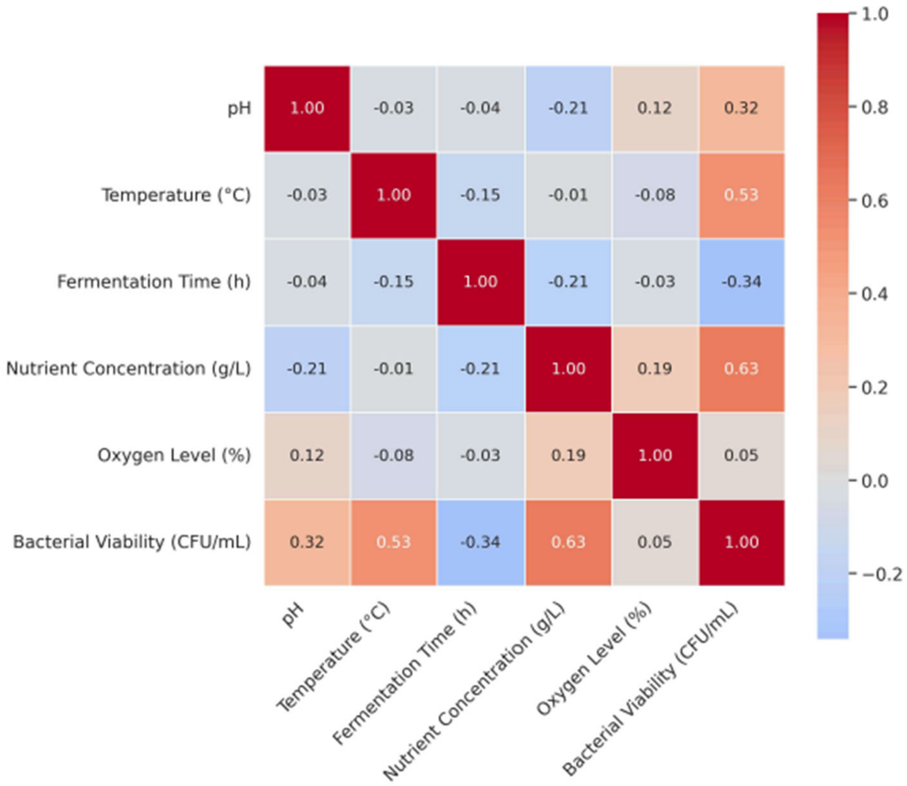

Figure 2. Correlation graph showing the relationship between critical variables in the inoculant production process.

The next step in the creation of the digital twin was the creation of a data-driven model using machine learning (ML) to identify patterns and predict outcomes. In this case, encoders were used. Encoder technology, particularly autoencoders, can be a powerful tool for modeling the inoculant production process in the context of ML. Using encoders or autoencoders is a viable and promising strategy to model the inoculant production process.

Among other ML models (e.g., LSTM for time-series data), autoencoders seem a better alternative for identifying the "normal" behavior of a system (like a golden batch). They learn the most relevant features from complex data by compressing it into a latent space, for example, to reduce dimensionality, detect anomalies, or understand underlying structures in high-dimensional process data.

Once the model is ready, it is possible to simulate production in real time and visualize the results. This is where Matplotlib and Seaborn come in handy again, along with more dynamic tools like Grafana. This way, interactive dashboards can be generated and make visible deviations from optimal behavior (e.g., temperature, pH, and substrate concentration), enabling timely corrective actions.

Then, Seaborn was used to visualize how certain parameters affect batch quality and ease metric validation from an autoencoder used for golden batch detection.

Finally, the solution was deployed in the productive environment. The system does not work in an autonomous way. In this case, the DT produces information for the operator to adjust the setup of the process to maintain optimal conditions. Then, the MVP produces information to predict future states of the system and provide optimal control actions by adjusting the feed rate or feed composition. This way, it can ensure consistent product quality.

3. Conclusions and Future Research

The case shows the power of the solution proposed through IIoT and DT. It shows that production management is simplified by having objective data to make decisions that allow the transition to excellence. Nevertheless, the challenge lies in moving from a conventional process to an intelligent process and being able to take the data from the process floor, including every event and sensor, to higher levels of information management. Ultimately, the goal is to develop a more empowered process operator to achieve better results. This is one of the key objectives of the model I5.0.

The implementation of the solution meant a joint effort between the company's process engineers, production experts, and data science and industrial digitalization professionals. The solution was achieved through an important co-creation process, in which each party contributed to its development; combined knowledge of the industrial domain and data generated a product with high added value aimed at improving processes and, collaterally, contributing to environmental sustainability. This issue should be considered; the successful adoption of a new solution requires compromise and maturity from the professionals of the adopting firm to reach the objectives of the digitalization process.

Regarding technical details for advancing data use, a deeper analysis can be conducted using libraries like Pyomo or CVXPY for more advanced optimization by providing more visibility regarding the variations in critical parameters. This point is scheduled to be the next step in the development of the solution once the adopted version is stabilized. Through these tools, a more complex analysis can be performed. Currently, the most relevant result is an optimization of the concentration, reducing about 10% of the bio materials and still meeting market requirements.

An important observation that should be highlighted is that integrating ML to train the behavioral model within a DT, as in the case to predict how certain parameters affect the quality of a batch, allows the system to be optimized both predictively and in real time, offering the best of both worlds. This way, operators have a complete picture to learn and understand the process for the best set. This case demonstrates how a digital twin can result in benefits by offering users the ability to use process and endpoint monitoring and control, continuous improvement, and a knowledge management tool in an integrated manner.

The result of the case study is a Minimum Viable Product (MVP) of a DT that demonstrates the power of the digital solution obtained by integrating siloed information through the IIoT architecture and then linking open-source software tools. The approach described in the case study validates the technology set chosen to achieve the solution by helping to reduce the consumption of biomaterials. Training data and cause-and-effect analysis can be significantly improved, offering batch predictions. The best batch performance can be achieved by exploring, discovering, prototyping, testing, tuning, justifying, deploying, commissioning, maintaining, and continuously improving the digital twin.

A last consideration is that IIoT and DTs should be recognized as key enablers in advancing the United Nations (UN) Sustainable Development Goals (SDGs) [28], particularly those focused on industrial innovation, responsible consumption and production, and climate action. Achieving high sustainability standards requires enhancing the technical and scientific quality of production systems, a goal that IIoT and DT technologies can significantly facilitate. This point contributes to the second key objective of Industry 5.0, which refers to the need to lower the impact of productive activities on the environment.

Author Contributions: Conceptualization, methodology, formal analysis, investigation, and writing—review and editing, F.W.M. Resources, visualization, supervision, project administration, and funding acquisition, A.R. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: The original contributions presented in this study are included in the article. Further inquiries can be directed to the corresponding authors.

Conflicts of Interest: The authors declare no conflict of interest.

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