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Is Your CDMO Using These AI-Driven Solutions In CMC For Oligos And Peptides?

By Kishore Hotha, Dr. Hotha's Life Sciences LLC

Artificial intelligence (AI) is revolutionizing biomanufacturing by addressing critical challenges, especially in scaling production. AI platforms anticipate and resolve bottlenecks by analyzing vast data sets to detect variability in real time. For example, AI-powered monitoring systems flag deviations in synthesis or purification processes, allowing immediate corrective actions. Predictive analytics further optimizes workflows by simulating manufacturing conditions, identifying potential issues, refining processes, and improving yields while minimizing costs. These innovations are instrumental in enabling manufacturers and their CDMO partners to scale confidently.

CDMOs play a crucial role in bridging the gap between R&D and commercialization. Biomanufacturers ask a lot of their CDMOs, such as meeting diverse expectations and navigating complex regulatory requirements. Meanwhile, oligonucleotides and peptides, pivotal in addressing complex diseases, require precise, scalable, and compliant production (see my earlier article, CMC Strategies With CDMOs: Ensuring CQAs For Oligos And Peptides). By integrating AI-driven technologies seamlessly to overcome chemistry, manufacturing, and controls (CMC) challenges, CDMOs are delivering robust, scalable solutions, transforming therapeutic development and commercialization. The following sections explore how these innovations drive operational excellence and advance the biomanufacturing landscape.

AI In Oligonucleotide Development

AI platforms such as Benchling, Labguru, and Sartorius' BioPAT are redefining how oligonucleotides are developed. These tools optimize phosphoramidite chemistry through predictive synthesis models, reducing errors like truncated sequences while improving coupling efficiency. High-resolution LC-MS systems powered by AI streamline impurity profiling, identifying and quantifying complex impurities with unprecedented speed and precision. Real-time monitoring systems like Siemens' MindSphere track synthesis in progress, flagging deviations in reagent quality or coupling efficiency, ensuring batch-to-batch consistency. Digital twins simulate large-scale manufacturing processes for scalability, providing actionable insights to refine workflows without physical trials. In addition, AI tools simplify regulatory compliance through automated documentation workflows and predictive analysis for post-approval changes, helping manufacturers stay ahead of regulatory demands.

AI In Peptide Development

Platforms like AlphaFold and IBM Watson are instrumental in addressing the complexities of peptide development. AlphaFold revolutionizes sequence optimization and folding predictions, ensuring peptides adopt bioactive conformations while minimizing immunogenicity risks. AI-driven tools simulate post-translational modifications (PTMs) like glycosylation, achieving consistency in large-scale manufacturing. Advanced dynamic light scattering (DLS) systems, integrated with AI, detect aggregation risks during formulation and mitigate them by suggesting real-time adjustments. Predictive algorithms assess environmental factors that could lead to peptide degradation or instability, accelerating the identification of stabilization strategies. AI-powered digital twins simulate manufacturing processes for scaling, while platforms like TetraScience streamline tech transfers, ensuring seamless transitions from R&D to commercial production.

AI For Effective CMC Development

Adopting AI transforms internal operations and strengthens customer centricity. Advanced AI platforms like Benchling, TetraScience, and Veeva Vault improve transparency, accelerate timelines, and enhance quality. These tools enable real-time project tracking, data sharing, and communication through dashboards that display metrics such as synthesis efficiency, batch consistency, and quality control results. Predictive analytics further builds trust by proactively identifying potential production delays and risks, allowing timely corrective actions. By leveraging AI to streamline collaboration and align with client goals, CDMOs deliver exceptional value, meeting client expectations while driving efficiency and operational excellence.

AI In Analytical Validation And Regulatory Excellence

Integrating AI technologies significantly enhances analytical validation, a crucial component in oligonucleotide and peptide development. Advanced platforms such as Veeva Vault and TetraScience accelerate stability testing by simulating extended storage conditions within a fraction of the time, enabling rapid identification of degradation pathways. Machine learning algorithms process high-resolution LC-MS

and DLS data to pinpoint impurities and contaminants, ensuring production batches maintain consistent quality. For regulatory adherence, automated systems streamline the preparation of submission-ready documents, monitor real-time regulatory updates, and evaluate the compliance impact of process modifications, minimizing administrative overhead while improving accuracy.

Regulatory Support With A Client-Centric Approach By CDMOs

CDMOs harness AI-powered regulatory tools like TetraScience and Veeva Quality One to simplify compliance processes. These platforms enable automation of documentation, real-time tracking of regulatory updates, and efficient management of post-approval changes. By providing clients with a transparent view of regulatory activities, CDMOs establish themselves as proactive collaborators, adept at navigating the complexities of compliance requirements while ensuring seamless execution.

Seamless Scaling With AI

With AI platforms such as GE's Predix and OSIsoft's PI System, scaling the production of oligonucleotides and peptides becomes significantly more efficient. These tools optimize reaction conditions, reagent concentrations, and manufacturing workflows to maximize yields while minimizing waste. Continuous manufacturing processes powered by real-time AI insights enable scalability without compromising quality. For peptides, AI ensures uniform PTM application and aggregation prevention during scale-up, leveraging tools like advanced molecular simulation software to maintain therapeutic efficacy.

Streamlining Proposal And Project Management

AI systems like Asana and Trello, integrated with machine learning algorithms, can automate resource allocation, timeline forecasting, and milestone tracking. CDMOs can leverage these tools to provide clients with accurate, dynamic project plans, ensuring they stay informed about progress and timelines. Platforms like Smartsheet, Airtable, and Wrike with AI features also can enhance proposal generation, tailoring cost and delivery timelines based on historical data and current project parameters. Additionally, tools like Jira and ClickUp offer advanced project tracking and agile management features, further optimizing the workflow for CDMOs.

Driving Quality, Flexibility, And Sustainability With AI

AI empowers CDMOs to deliver superior quality, adapt to client demands, and embrace sustainable practices. Tools like Sartorius' BioPAT and OSIsoft's PI System ensure batch-to-batch consistency and reduce variability, fostering confidence in reliable production. AI-powered LC-MS systems accelerate impurity and stability reporting, enabling timely client decisions.

Advanced platforms such as Siemens' MindSphere and digital twin technology streamline process simulations for oligonucleotides and peptides, ensuring seamless scaling and avoiding costly delays. By modeling production scenarios, CDMOs gain the flexibility to address client requests for additional batches or process changes efficiently.

Custom solutions through AI platforms like Amazon SageMaker and Azure Machine Learning cater to specific client needs, optimizing synthesis processes or addressing peptide aggregation risks. These tailored approaches enhance client satisfaction and build enduring partnerships.

Additionally, AI drives eco-friendly production by minimizing waste and energy consumption. Tools like AspenTech optimize chemical processes to balance environmental responsibility with cost efficiency, meeting the growing demand for sustainable manufacturing practices. By leveraging these innovations, CDMOs enhance operational efficiency while aligning with client priorities and regulatory expectations.

AI As A Catalyst For Transforming Therapeutic Development

Incorporating AI is revolutionizing the CMC landscape for oligonucleotides and peptides, enabling deeper client relationships and fostering customer-centric operations. AI empowers CDMOs to address unique challenges while maintaining operational excellence by enhancing transparency, accelerating timelines, and streamlining processes.

AI improves synthesis, scalability, and regulatory compliance, driving sustainability and innovation. It bridges R&D and manufacturing, strengthens partnerships, and future-proofs the development of complex therapies. This transformative integration ensures the delivery of high-quality, scalable therapeutics that meet the evolving needs of patients and industry.

Key Software Platforms And Their Applications/Functions In AI-Driven CMC Development

Synthesis and Optimization Tools

- **Benchling**: Synthesis optimization and project tracking.
- **Labguru**: Predictive synthesis and data management.
- **AspenTech**: Sustainable and efficient chemical processes.
- **PeptiSoft**: Designed specifically for peptide and oligonucleotide synthesis.
- **RFpeptides**: AI-driven tool for designing bioactive peptides.

Analytical and Quality Control Tools

- **Sartorius' BioPAT**: Impurity profiling and quality control.
- **Siemens' MindSphere**: Process monitoring and simulations.
- **AlphaFold**: Peptide folding predictions.
- **IBM Watson**: Post-translational modifications and stabilization.
- **TetraScience**: Regulatory compliance and analytics.

Workflow and Data Management Tools

- **Veeva Vault**: Stability testing and documentation automation.
- **GE's Predix**: Workflow and reaction optimization.
- **OSIsoft's PI System**: Continuous manufacturing insights.

Project Management and Resource Allocation Tools

- **Asana, Trello, Smartsheet**: Project management and resource allocation.
- **Wrike, Jira, ClickUp**: Proposal generation and project tracking.

AI and Machine Learning Tools

- **Amazon SageMaker**: Custom AI for synthesis and aggregation risks.
- **Azure Machine Learning**: Tailored AI applications.

About The Author:

Kishore Hotha, Ph.D., is the president of Dr. Hotha's Life Sciences LLC, a global consulting firm, and is a scientific and business leader in the pharmaceutical biotech and CDMO sectors, spanning drug development from early-stage research to commercialization. He has made significant contributions to numerous IND, NDA, and ANDA submissions for drug substances and products across small and large molecules, including ADCs, oligonucleotides, and peptides, through commercialization. Hotha holds a Ph.D. from JNT University and an MBA from SNHU. Previously, he served as the global VP at Veronova and global director at Johnson Matthey, with pivotal roles at Lupin and Dr. Reddy's. Hotha has contributed to over 80 publications and serves on various editorial boards.