News and Perspectives

AI-Designed Radiopharmaceuticals: How Machine Learning Is Redefining Precision Cancer Therapy

Benedette Cuffari, JMIR Correspondent

Abstract

Computing advances are helping improve the precision and effectiveness of cancer treatment. In this *News and Perspectives* article, JMIR Correspondent Benedette Cuffari reports on recent AI applications for radiopharmaceutical therapy, as well as the current state of the field and its future potential.

Key Takeaways:

- Radiopharmaceutical therapy may offer more targeted treatment for some types of cancer, with the potential to reduce radiation exposure and damage to healthy tissues, although it is time- and resource-intensive to develop.
- Compared to traditional development methods, deep learning and generative AI models can more rapidly identify novel targets and engineer highly stable radiopharmaceuticals with less expense.
- The lack of standardized, high-quality data to train and generalize these frameworks limits widespread clinical adoption.

In oncology, radiation therapy uses an external source of radiation that delivers high-energy X-rays, protons, or electron beams from outside the body to destroy cancer cells. Comparatively, radiopharmaceutical therapy involves typically intravenous (IV) administration of radioactive molecules that enter tumors by targeting specific types of cells. Inside the cell, radiopharmaceuticals undergo radioactive decay; as these drugs are broken down, they release radiation in the form of alpha or beta energy that damages cancer DNA and causes cell death. It can be more effective—and less damaging—for identifying and treating some types of cancer.

Today, 67 radiopharmaceuticals are approved worldwide, 54 of which are used for diagnostic purposes. The remaining 13 radiopharmaceuticals are used to treat cancer, either alone or in combination with chemotherapy and surgery. Despite their established efficacy, radiopharmaceuticals are associated with numerous limitations related to their safety and ability to effectively reach tumors.

Addressing these challenges requires carefully optimizing the physical and biological properties of radiopharmaceuticals. These efforts can involve adjusting how the radioactive substance is attached to targeting molecules that bind to tumor cells and how stable it is in the body. Research in this area also examines how different strategies can be adopted to more effectively locate and bind to cancer cells and avoid healthy tissues, thereby improving treatment outcomes and reducing side effects.

Recent advances in AI technologies are revolutionizing nuclear medicine, with the potential to improve the specificity of radiopharmaceutical targeting while reducing safety concerns. If successful, AI has the potential to shorten the amount of time needed to develop new radiopharmaceuticals, identify specific treatments that are most likely to prevent cancer recurrence, and reduce radiation exposure to healthy tissues.

AI-Powered Discovery and Design

According to Sofia Michopoulou, PhD, a medical physics expert who leads Nuclear Medicine Physics at University Hospital Southampton, AI has the potential to significantly accelerate the discovery pipeline by enabling the design and evaluation of new pharmaceuticals using computer simulations.

“This may help identify the most promising pharmaceutical candidates earlier, reduce the current volume of preclinical work, and make early-phase evaluation more focused and efficient,” she says.

During radiopharmaceutical drug design, deep learning (DL) models can be used to predict how specific chemical changes may influence how these drugs behave in human patients. New versions of AlphaFold, an AI protein structure database developed by Google DeepMind, more accurately predict how drug candidates interact with proteins and genetic material. When combined with patient-specific data, these models can help identify and prioritize targets that are more likely to be effective and spread appropriately in the body.

Generative adversarial networks (GANs) and related tools have been proposed to virtually design and test thousands of potential drug structures before synthesizing them. For example, generative AI models can suggest changes to a drug’s chemical structure to help it bind more precisely to its target and remain stable during radioactive decay.

Predicting Biodistribution and Dosimetry

Accurately predicting the dose of radiation that will be absorbed is an essential aspect of radiopharmaceutical therapy to maximize the amount of radiation delivered to tumors while minimizing radiation exposure to healthy tissues.

Typically, organ-level dosimetry calculations based on average anatomical models, rather than patient-specific anatomy, are widely used. These models are associated with numerous limitations. They assume that radiopharmaceuticals are uniformly distributed in a target organ or tissue and don’t fully account for the fact that patients may have anatomical differences or respond differently to the same drug, or that there can be uneven uptake within tumors.

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> Sofia Michopoulou, PhD

DL models can improve the precision of these dose calculations. For example, specific AI models—3D convolutional neural networks (CNNs)—have been developed to analyze medical images and predict how radiation will be distributed across tissues, with some outperforming traditional methods. Machine learning (ML), particularly DL, has also been used to generate digital twins that support personalized dose calculations and treatment planning before radiopharmaceutical therapy.

Michopoulou believes this represents one of the most promising areas of convergence between AI and nuclear medicine.

“The most exciting prospect is personalized theranostics supported by digital twins,” she says. “By combining molecular imaging, radiopharmaceutical therapy, and patient-specific modeling, we could optimize treatment for each individual patient, rather than relying on standardized approaches.”

Beyond direct dose estimation, DL techniques like super-resolution modeling and noise reduction can improve the quality and details of positron emission tomography (PET) images without exposing the patient to additional radiation. The integration of these high-quality PET images with kinetic modeling could further improve patient-specific estimates of how radiation will be distributed and individualize therapeutic doses.

Early Successes

Several GAN-based systems trained and tested on data from both synthetic images and human patients have been evaluated, with these studies supporting the potential clinical application of these models.

For example, one DL-based method has been used to create later-stage PET scan images from earlier scans to predict how patients will respond to treatment, as well as to reduce the need for additional scans after radiopharmaceutical administration.

CNN-based models that identify and outline tumors in medical images have also improved the precision of radiation dose calculations by more accurately identifying tumor boundaries. Integrating data about how these drugs move through the body into these models has further improved the accuracy of predicted doses delivered to critical organs like the kidneys, liver, spleen, and salivary glands to reduce harmful side effects.

AI-driven tools are increasingly becoming part of routine clinical workflows in radiopharmaceutical therapy. Michopoulou continues, “AI is now used extensively for image segmentation, greatly accelerating [the] speed of data preparation for dosimetry. It is also increasingly being introduced into image reconstruction, which is exciting and also comes with new validation challenges, influencing treatment decisions.”

Barriers to Clinical Translation

Implementing AI tools in radiopharmaceutical discovery and development remains challenging. Data can be hard to come by, models may not always generalize appropriately, and there are ethical concerns around data ownership and confidentiality to consider. Some of these challenges may be addressed with federated learning—allowing models at different hospital sites to share what they’ve learned to ensure the diversity of available data without sharing patient-specific information.

But without enough systematic, standardized data to train these AI models, they’re limited in how accurate and widely applicable they can be. Addressing this limitation will require extensive foundational experimental research. Complementary efforts to standardize datasets used to train and optimize DL models for tasks like organ segmentation are essential for reliable dose calculations and should be prioritized to accelerate clinical adoption.

Although these significant technical and regulatory challenges remain, AI is increasingly being incorporated into every stage of radiopharmaceutical development. These advances are supporting more personalized approaches to cancer care while improving patient outcomes and treatment planning.

Keywords: radiopharmaceuticals; theranostics; deep learning; personalized medicine; radioligand discovery

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