

# The Future Prospect of Integrating Machine Learning and Nanocarbon Materials in Cancer Treatment: A Prospective Review

Luiz Fernando Romanholo Ferreira

Graduate Program in Genomic Sciences and Biotechnology, Catholic University of Brasília, Brasília, 71966-700, Brazil

Corresponding author's e-mail: [luiz.romanholo@p.ucb.br](mailto:luiz.romanholo@p.ucb.br)

## Article Information

Received: 20 May 2025  
Revised: 31 May 2025  
Accepted: 01 June 2025  
Published online: 07 June 2025

## Keywords

Artificial intelligence  
Cancer treatment  
Drug delivery  
Machine learning  
Nanocarbon  
Nanotechnology

## Abstract

Cancer, as one of the leading causes of global mortality, requires novel therapeutic approaches with high efficiency and low side effects. In this regard, combining artificial intelligence (AI), particularly machine learning (ML), with nanocarbon materials such as carbon nanotubes and graphene has brought new hope. Hence, this review aims to investigate the role of ML in optimizing diagnosis, predicting treatment response, and designing smart nanocarriers based on nanocarbon. Nanotechnology and AI enable targeted drug delivery, photothermal therapy, and more accurate imaging. For example, carbon nanoparticles can deliver chemotherapy drugs directly to tumors, while ML predictive models analyze medical images to accurately assess a patient's response to treatment and recommend the best course of action. This convergence of technologies has opened up new hopes for the fight against cancer. However, there are challenges, such as the potential toxicity of nanocarbons, the need for extensive clinical data to train ML models, and integrating these technologies into therapeutic systems. In the future, the development of smarter nanocarriers, aided by machine learning and further studies on the biocompatibility of nanocarbons, could lead to more personalized and effective therapies. In conclusion, the integration of ML and nanocarbons has the potential to revolutionize oncology, but interdisciplinary research and large-scale clinical trials are necessary to achieve practical application.

© 2025 University of Zabol. All rights reserved.

## 1. Introduction

Each year, millions of people all over the world lose their lives to cancer, as it is one of the most complex and deadly diseases of our time [1, 2]. Despite the relative effectiveness of conventional treatment methods such as chemotherapy, immunotherapy, and radiotherapy, there are many side effects associated with them, and they may

cause damage to healthy cells as well [3-5]. As a result of these limitations, researchers have developed new technologies to overcome them. Nanotechnology, particularly carbon nanomaterials, has opened up new opportunities for targeting cancer treatments due to their unique physical and chemical characteristics [6, 7].

Nanomaterials such as carbon nanotubes, graphene, and carbon dots possess many desirable characteristics that make them ideal tools for the delivery of drugs, the imaging of cancer cells, and the selective destruction of cancer cells, because they are very small, have a high specific surface area, and can be modified chemically [8, 9]. Carbon nanotubes can deliver drugs directly to cancerous tissues, preventing drug degradation in the bloodstream and enabling controlled drug release via optical or magnetic stimulation [10, 11].

Personalized medicine withered before recent advances in AI, particularly ML [12]. ML algorithms make it possible to analyze large amounts of clinical data to identify complex disease patterns, predict treatment responses, and design optimal treatment strategies [13, 14]. This technology can also alleviate the challenges associated with using nanocarriers.

By combining AI and carbon nanotechnology, a comprehensive approach can be taken to overcome cancer treatment limitations promptly. It is possible to produce smart nanocarriers by integrating these two technologies, optimizing treatment parameters, and reducing the risk of side effects through their combination. Despite the progress made in this field, significant challenges remain, including the potential toxicity of nanomaterials and the need for accurate clinical data. Therefore, this review examines the application of ML for optimizing diagnosis, predicting treatment response, and designing intelligent nanocarriers that utilize nanocarbon as the material for carrier synthesis.

## 2. Machine Learning in Cancer Treatment

ML algorithms have revolutionized cancer diagnosis and treatment [15, 16]. Advanced ML models can accurately predict patients' treatment responses, including chemotherapy and radiation, by analyzing complex genomics, proteomics, and medical imaging datasets [17-19]. For instance, Deep Neural Networks (DNNs) can predict whether or not cancer patients will overcome drug resistance in the future [20-22]. Optimizing anticancer drug dosage is one of the most critical applications of ML. Calculating the most precise therapeutic dose using reinforcement learning algorithms (RL) that consider multiple parameters, such as a patient's age, genetic status, treatment history, and side effects, is possible [23, 24]. As a result of this technology, combination chemotherapy is beneficial (Figure 1) [25].

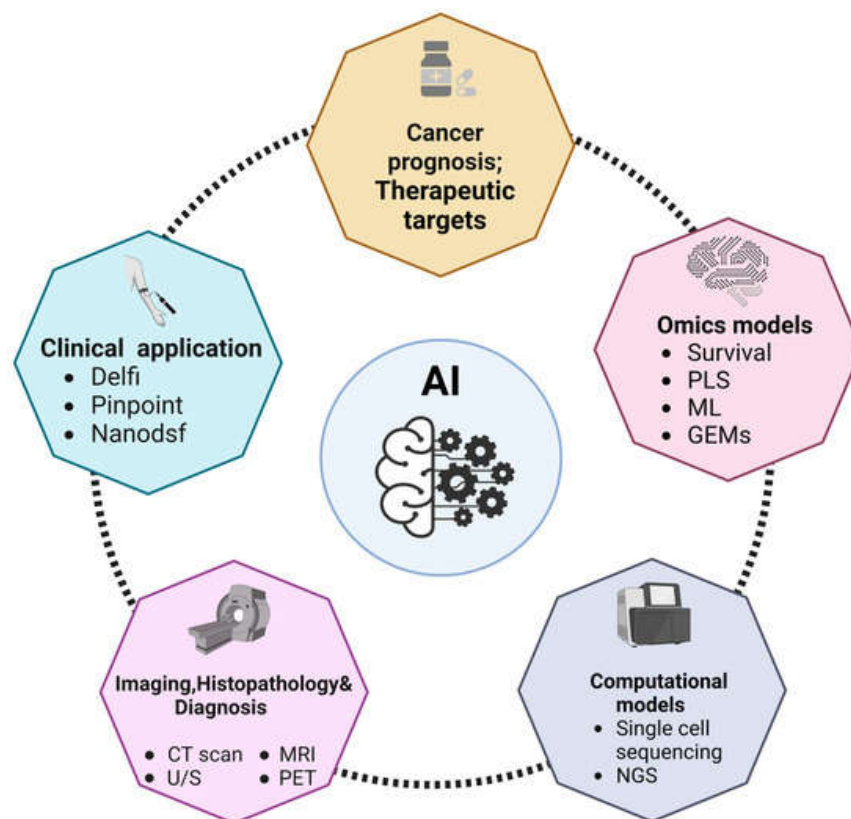
ML-based image processing algorithms have revolutionized radiology for earlier detection and better diagnosis in the field [26]. Intelligent systems can detect highly sensitive tumors by analyzing images such as computed tomography (CT) scans, magnetic resonance imaging (MRI), and mammography scans [27, 28]. With advanced techniques such as transfer learning, models can perform well even with limited training data. One of the latest developments in this area of research involves the development of models for predicting tumor progression and metastatic spread. In the case of hybrid ML models incorporating data from multimodal imaging and genetic information, it is possible to model tumor growth patterns more accurately than ever [29, 30].

## 3. Carbon Nanomaterials in Cancer Treatment

Nanotechnology, one of the most advanced and innovative scientific branches in recent decades, has led to a fundamental transformation in the field of medicine. As a result, many methods of diagnosing, treating, and even

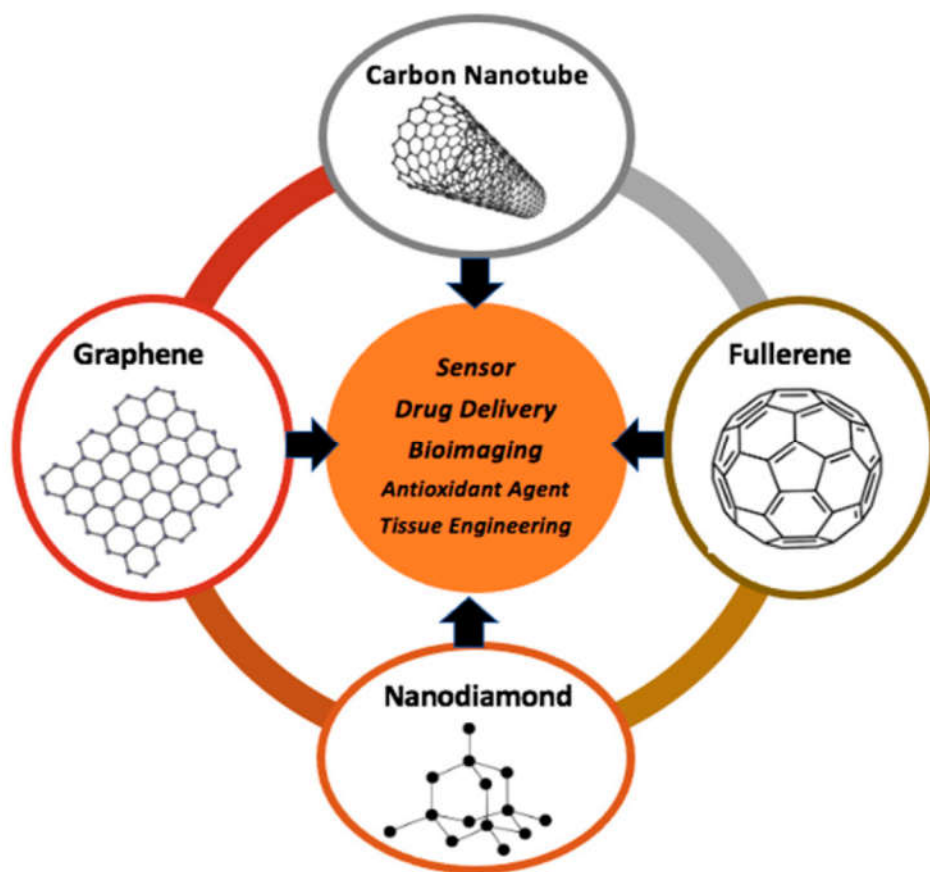
---

preventing diseases have achieved unprecedented accuracy and efficiency through the application of nanotechnology [31-36]. Due to their unique physicochemical properties, carbon nanomaterials have revolutionized drug delivery [37, 38]. Carbon nanoparticles, such as nanotubes and graphene oxide, possess numerous advantages due to their high specific surface area and adaptability in modifying the structure of their functional groups [39-41]. By binding particular ligands, such as anti-epidermal growth factor receptor antibodies, carbon nanocarriers can transport drugs directly to cancer cells [42].



**Figure 1.** Overview of the applications of AI to cancer diagnosis and the oncology research field. The scheme depicts the main fields of AI application discussed in this review. Abbreviations: computed tomography, CT; gene expression models, GEMs; machine learning, ML; magnetic resonance imaging, MRI; nano differential scanning fluorimetry, Nanodsf; next-generation sequencing, NGS; positron emission tomography, PET; partial least squares analysis, PLS; ultrasound imaging, U/S [25]

Carbon dots have been proposed as a next-generation contrast agent in medical imaging [43-45] (Figure 2). In addition to high quantum yields, these nanostructures are also excellent for photostability [46]. By crossing the blood-brain barrier, carbon dots can produce nanometer-resolution imaging of cancerous tissues by selectively accumulating in those tissues where cancer is present [47, 48]. Among recent research efforts, hybrid nanocarriers have been developed. It is possible to fabricate hybrid graphene-gold nanoparticles that can simultaneously deliver drugs, perform photothermal therapy, and enable imaging [49-51]. Using these multifunctional systems, precise imaging, therapeutic effect, and real-time monitoring of therapeutic response can all be provided simultaneously as part of a single device. The primary challenge in this area is achieving improved biocompatibility and clearance of these nanomaterials from the body once their function is complete, a topic that has been the subject of extensive research in this field.



**Figure 2.** Schematic summary of nanocarbon material for various pharmaceutical applications [45]

#### 4. Combining ML and Nanocarbons for Smart Cancer Therapy

In the field of cancer therapy, the combination of ML and nanocarbon technology has created a new paradigm [52, 53]. Using advanced deep learning algorithms, carbon nanoparticle structures can be designed with atomic precision and optimized for drug release properties [54-56]. Generative Adversarial Networks (GANs) are one way to encapsulate drugs in nanographene structures with controlled porosity to release them according to specific stimuli, such as pH or temperature [57, 58].

Using ML algorithms, it is possible to predict the metabolic pathways of cancer cells after contact with nanoparticles by analyzing microscopic and spectroscopic information as a result of modeling nanoparticle-cell interactions [59-61]. In the case of nanoparticles, CNNs offer spatially high accuracy in determining how nanoparticles penetrate tumors [62, 63]. Researchers can design nanocarriers with the maximum ability to collect cancer cells and the least amount to capture healthy cells. This is with the help of these advances. As a result of this technology integration, it is also possible to optimize therapeutic parameters, which is another key application. ML algorithms can help adjust critical parameters in photothermal therapy, such as the intensity of laser irradiation, the concentration of therapeutic drugs, and the real-time timing of medication injection [57, 64]. This technology has been revolutionary, especially in treating tumors resistant to particular chemotherapy types. Recent breakthroughs in this field have included the development of self-learning systems for designing fourth-generation nanocarriers (Table 1).

**Table 1.** AI algorithms in nanocarbon-based cancer therapy

AI Algorithm	Application in Cancer Treatment	Role of Nanocarbons
<b>Convolutional Neural Networks</b>	Tumor detection & segmentation in medical imaging (MRI, CT scans)	Nanocarbon-enhanced contrast agents improve imaging accuracy
<b>Random Forest</b>	Predicting patient response to chemotherapy/immunotherapy	Nanocarriers deliver drugs, while AI optimizes dosage based on predictions
<b>Support Vector Machines</b>	Classifying cancer subtypes based on genomic data	Nanosensors collect high-precision biomarker data for AI analysis
<b>Reinforcement Learning</b>	Optimizing dynamic treatment plans (adaptive radiotherapy)	Nanoprobes monitor tumor changes in real time, feeding data to AI for adjustments
<b>Deep Reinforcement Learning</b>	Autonomous drug discovery & nanomedicine design	AI designs nanocarbon structures for targeted drug delivery
<b>Natural Language Processing</b>	Extracting insights from clinical reports & research papers	Integrates nanocarbon-based trial data into AI knowledge bases

## 5. Challenges and Future Prospects

Although significant progress has been made in developing these technologies, there are still substantial challenges to commercialization. Safety concerns prevent nanocarbon use. Carbon nanotubes may cause oxidative stress in the body and inflammation in the tissues in some cases. An innovative coating and surface modification method using ML can be developed to overcome this challenge. Several algorithms can be used to predict toxicity, such as identifying safer structures.

The other challenge is the need for high-quality clinical data to evaluate this novel treatment. As a result, thousands of carefully annotated clinical samples must be collected to effectively train ML models. To address this issue, integrated databases of medical images, genomic data, and treatment outcomes can be created. Furthermore, semi-supervised and transfer learning techniques can also be used to reduce training data requirements.

To successfully integrate these advanced technologies into clinical systems, AI experts, nanotechnologists, and clinicians must collaborate at a level that has never been seen before. User-friendly platforms for software development that can make these technologies understandable to clinical professionals are needed, and this is a future priority for research. Ultimately, these technologies will be widely adopted if the treatment protocols are standardized and appropriate regulatory frameworks are established to ensure their wide acceptance.

## 6. Conclusion

Combining ML with nanocarriers has revolutionized personalized cancer treatment in recent years. Combining these two technologies enables the design of intelligent therapeutic systems that can dynamically adapt to the unique characteristics of each patient and tumor by optimizing nanocarriers. As a result of this convergence of technology, AI can predict the treatment outcome accurately. Nanotechnology and AI will play a crucial role in the future of cancer treatment by combining intelligent multimodal approaches that complement each other.

## Conflicts of Interest

The author declares no conflict of interest associated with this manuscript.

## Declaration of the Use of Generative AI

After the content was fully written, an AI-powered tool was exclusively used to review and refine the manuscript's grammar, punctuation, and overall linguistic flow. The AI tool was used strictly as a proofreading and language refinement assistant and was not employed at any stage for generating content, ideas, or writing chapter sections.

## References

1. Obeagu EI, Obeagu GU. Breast cancer: A review of risk factors and diagnosis. *Medicine* 2024, 103(3), e36905.
2. Bizuayehu HM, Ahmed KY, Kibret GD, Dadi AF, Belachew SA, Bagade T, Tegegne TK, Venchiarutti RL, Kibret KT, Hailegebireal AH, Assefa Y. Global disparities of cancer and its projected burden in 2050. *JAMA Netw. Open* 2024, 7(11), e2443198.
3. Dagar G, Gupta A, Shankar A, Chauhan R, Macha MA, Bhat AA, Das D, Goyal R, Bhoriwal S, Pandita RK, Prasad CP. The future of cancer treatment: Combining radiotherapy with immunotherapy. *Front. Mol. Biosci.* 2024, 11, 1409300.
4. Natarelli N, Aleman SJ, Mark IM, Tran JT, Kwak S, Botto E, Aflatooni S, Diaz MJ, Lipner SR. A review of current and pipeline drugs for treatment of melanoma. *Pharmaceuticals* 2024, 17(2), 214.
5. Peer D, Karp JM, Hong S, Farokhzad OC, Margalit R, Langer R. Nanocarriers as an emerging platform for cancer therapy. In *Nano-enabled medical applications*, Balogh LP (Ed.), 2020, Jenny Stanford Publishing: Singapore, pp. 61-91.
6. Sadr S, Rahdar A, Pandey S, Hajjafari A, Soroushianfar M, Sepahvand H, Sasani B, Salimpour Kavasebi S, Borji H. Revolutionizing Cancer Detection: Harnessing Quantum Dots and Graphene-Based Nanobiosensors for Lung and Breast Cancer Diagnosis. *BioNanoScience* 2025, 15(1), 111.
7. Hajjafari A, Sadr S, Rahdar A, Bayat M, Lotfalizadeh N, Dianaty S, Rezaei A, Moghaddam SP, Hajjafari K, Simab PA, Kharaba Z. Exploring the integration of nanotechnology in the development and application of biosensors for enhanced detection and monitoring of colorectal cancer. *Inorg. Chem. Commun.* 2024, 164, 112409.
8. Paramasivam G, Palem VV, Meenakshy S, Suresh LK, Gangopadhyay M, Antherjanam S, Sundramoorthy AK. Advances on carbon nanomaterials and their applications in medical diagnosis and drug delivery. *Colloids Surf. B.* 2024, 241, 114032.
9. Kumar P, Pandey SN, Ahmad F, Verma A, Sharma H, Ashique S, Bhattacharyya SP, Bhattacharyya I, Kumar S, Mishra N, Garg A. Carbon nanotubes: a targeted drug delivery against cancer cell. *Curr. Nanosci.* 2024, 20(6), 769-800.
10. Pandey VK, Tripathi A, Taufeeq A, Dar AH, Samrot AV, Rustagi S, Malik S, Bhattacharya T, Kovacs B, Shaikh AM. Significance and applications of carbon dots in anti cancerous nanodrug conjugate development: A review. *Appl. Surf. Sci. Adv.* 2024, 19, 100550.
11. Akmal MH, Kalashgrani MY, Mousavi SM, Rahmanian V, Sharma N, Gholami A, Althomali RH, Rahman MM, Chiang WH. Recent advances in synergistic use of GQD-based hydrogels for bioimaging and drug delivery in cancer treatment. *J. Mater. Chem. B* 2024, 12(21), 5039-5060.
12. Rai HM. Cancer detection and segmentation using machine learning and deep learning techniques: A review. *Multimed. Tools Appl.* 2024, 83(9), 27001-27035.

13. MunishKhanna, Singh LK, Garg H. A novel approach for human diseases prediction using nature inspired computing & machine learning approach. *Multimed. Tools Appl.* 2024, 83(6), 17773-17809.
  14. Javed R, Abbas T, Khan AH, Daud A, Bukhari A, Alharbey R. Deep learning for lungs cancer detection: a review. *Artif. Intell. Rev.* 2024, 57(8), 197.
  15. Sherani AMK, Khan M, Qayyum MU, Hussain HK. Synergizing AI and Healthcare: Pioneering advances in cancer medicine for personalized treatment. *Int. Multidiscip. Sci. Arts* 2024, 3(2), 270-277.
  16. Singh AP, Saxena R, Saxena S, Maurya NK. Artificial intelligence revolution in healthcare: Transforming diagnosis, treatment, and patient care. *Asian J. Adv. Res.* 2024, 7(1), 241-263.
  17. Khan M, Shiwani A, Qayyum MU, Sherani AMK, Hussain HK. Revolutionizing Healthcare with AI: Innovative Strategies in Cancer Medicine. *Int. Multidiscip. Sci. Arts.* 2024, 3(2), 316-324.
  18. Odah M. Artificial Intelligence (AI) and Machine Learning (ML) in Diagnosing Cancer: Current Trends. (Preprint) 2024, 2024030433.
  19. Khan M, Shiwani A, Qayyum MU, Sherani AMK, Hussain HK. AI-powered healthcare revolution: an extensive examination of innovative methods in cancer treatment. *BULLETJ. Multidisip. Ilmu* 2024, 3(1), 87-98.
  20. Hajim WI, Zainudin S, Daud KM, Alheeti K. Optimized models and deep learning methods for drug response prediction in cancer treatments: a review. *PeerJ Comput. Sci.* 2024, 10, e1903.
  21. Liu Y, Shi J, Liu W, Tang Y, Shu X, Wang R, Chen Y, Shi X, Jin J, Li D. A deep neural network predictor to predict the sensitivity of neoadjuvant chemoradiotherapy in locally advanced rectal cancer. *Cancer Lett.* 2024, 589, 216641.
  22. Tyagi E, Kumari P, Prakash A, Bhuyan R. Revolutionizing Anti-Cancer Drug Discovery: The Role of Artificial Intelligence. *Int. J. Bioinform. Intell. Comput.* 2025, 4(1), 1-38.
  23. Teplytska O, Ernst M, Koltermann LM, Valderrama D, Trunz E, Vaisband M, Hasenauer J, Fröhlich H, Jaehde U. Machine Learning Methods for Precision Dosing in Anticancer Drug Therapy: A Scoping Review. *Clin. Pharmacokinet.* 2024, 63(9), 1221-1237.
  24. Ekundayo F. Reinforcement learning in treatment pathway optimization: A case study in oncology. *Int. J. Sci. Res. Arch.* 2024, 13(02), 2187-2205.
  25. Fawaz A, Ferraresi A, Isidoro C. Systems biology in cancer diagnosis integrating omics technologies and artificial intelligence to support physician decision making. *J. Pers. Med.* 2023, 13(11), 1590.
  26. Asif S, Wenhui Y, ur-Rehman S-, ul-ain Q-, Amjad K, Yueyang Y, Jinhai S, Awais M. Advancements and prospects of machine learning in medical diagnostics: unveiling the future of diagnostic precision. *Arch. Comput. Methods Eng.* 2025, 32, 853-883.
  27. Hussain D, Al-Masni MA, Aslam M, Sadeghi-Niaraki A, Hussain J, Gu YH, Naqvi RA. Revolutionizing tumor detection and classification in multimodality imaging based on deep learning approaches: Methods, applications and limitations. *J. X-Ray Sci. Technol.* 2024, 32(4), 857-911.
  28. Theja N, Pushpa V, Kumar S, Siva SS. Exploring the Frontiers of Machine Learning in Radiology: A Comprehensive Review of Applications, Advancements, and the Challenges that Lie Ahead. *Biosci. Biotechnol. Res. Asia* 2025, 22(1), 95-102.
  29. Nakach F-Z, Idri A, Goceri E. A comprehensive investigation of multimodal deep learning fusion strategies for breast cancer classification. *Artif. Intell. Rev.* 2024, 57(12), 327.
-

30. Zhou H, Zhou F, Zhao C, Xu Y, Luo L, Chen H. Multimodal data integration for precision oncology: Challenges and future directions. (Preprint) 2024, 240619611.
  31. Ahmar H. Nonenzymatic electrochemical detection of glucose using screen-printed electrode modified with Pd–Au nanoparticles encapsulated on dendrimer grafted multi-wall carbon nanotubes. *Curr. Appl. Sci.* 2024, 2(2), 67-78.
  32. Badehian HA, Badehian Z, Fatahpor A. The Effect of Stone-Wales Defect on the Geometrical Parameters and Electronic Properties of ACNTs (14, 14). *Curr. Appl. Sci.* 2023, 1(2), 79-84.
  33. Badehian HA, Badehian Z, Sharifirad R. Structural and Electronic Properties of Armchair Silicon Carbide Nanoribbon. *Curr. Appl. Sci.* 2023, 1(1), 51-58.
  34. Sadr S, Poorjafari Jafroodi P, Haratizadeh MJ, Ghasemi Z, Borji H, Hajjafari A. Current status of nanovaccinology in veterinary medicine science. *Vet. Med. Sci.* 2023, 9(5), 2294-2308.
  35. Dadwal A, Baldi A, Kumar Narang R. Nanoparticles as carriers for drug delivery in cancer. *Artif. Cells Nanomed. Biotechnol.* 2018, 46(sup2), 295-305.
  36. Salimi S, Badehian HA, Badehian Z. Phonon Spectra of Monolayer Silicon Carbide. *Curr. Appl. Sci.* 2023, 1(2), 91-96.
  37. Sonowal L, Gautam S. Advancements and challenges in carbon nanotube-based drug delivery systems. *Nano-Struct. Nano-Objects* 2024, 38, 101117.
  38. Jadhav V, Roy A, Kaur K, Rai AK, Rustagi S. Recent advances in nanomaterial-based drug delivery systems. *Nano-Struct. Nano-Objects* 2024, 37, 101103.
  39. Malode SJ, Pandiaraj S, Alodhayb A, Shetti NP. Carbon nanomaterials for biomedical applications: progress and outlook. *ACS Appl. Bio Mater.* 2024, 7(2), 752-777.
  40. Parvin N, Kumar V, Joo SW, Mandal TK. Emerging trends in nanomedicine: carbon-based nanomaterials for healthcare. *Nanomater.* 2024, 14(13), 1085.
  41. Sadr S, Nazemian S, Dianaty S, Hajjafari A, Fazel B, Rezaei A, Rahdar A, Fathi-Karkan S, Bayat M, Pandey S, Franco OL. Advancing gut microbiome insights: Graphene quantum dot nanobiosensors for microbial metabolite detection. *Chem. Eng. J.* 2025, 513, 162954.
  42. Spada A, Gerber-Lemaire S. Surface Functionalization of Nanocarriers with Anti-EGFR Ligands for Cancer Active Targeting. *Nanomater.* 2025, 15(3), 158.
  43. Ghosal K, Ghosh A. Carbon dots: The next generation platform for biomedical applications. *Mater. Sci. Eng. C* 2019, 96, 887-903.
  44. Boakye-Yiadom KO, Kesse S, Opoku-Damoah Y, Filli MS, Aquib M, Joelle MM, Farooq MA, Mavlyanova R, Raza F, Bavi R, Wang B. Carbon dots: Applications in bioimaging and theranostics. *Int. J. Pharm.* 2019, 564, 308-317.
  45. Jiwanti PK, Wardhana BY, Sutanto LG, Dewi DM, Putri IZ, Savitri IN. Recent development of nano-carbon material in pharmaceutical application: a review. *Molecules* 2022, 27(21), 7578.
  46. Jia Q, Zhao Z, Liang K, Nan F, Li Y, Wang J, Ge J, Wang P. Recent advances and prospects of carbon dots in cancer nanotheranostics. *Mater. Chem. Front.* 2020, 4(2), 449-471.
  47. Chung YJ, Kim J, Park CB. Photonic carbon dots as an emerging nanoagent for biomedical and healthcare applications. *ACS Nano* 2020, 14(6), 6470-6497.
-

48. Mhlanga N, Mphuthi N, Van der Walt H, Nyembe S, Mokhena T, Sikhwivhilu L. Nanostructures and nanoparticles as medical diagnostic imaging contrast agents: A review. *Mater. Today Chem.* 2024, 40, 102233.
  49. Yang L, Kim TH, Cho HY, Luo J, Lee JM, Chueng ST, Hou Y, Yin PT, Han J, Kim JH, Chung BG. Hybrid graphene-gold nanoparticle-based nucleic acid conjugates for cancer-specific multimodal imaging and combined therapeutics. *Adv. Funct. Mater.* 2021, 31(5), 2006918.
  50. Al-Ani LA, AlSaadi MA, Kadir FA, Hashim NM, Julkapli NM, Yehye WA. Graphene-gold based nanocomposites applications in cancer diseases; Efficient detection and therapeutic tools. *Eur. J. Med. Chem.* 2017, 139, 349-366.
  51. Gao S, Zhang L, Wang G, Yang K, Chen M, Tian R, Ma Q, Zhu L. Hybrid graphene/Au activatable theranostic agent for multimodalities imaging guided enhanced photothermal therapy. *Biomater.* 2016, 79, 36-45.
  52. Chugh V, Basu A, Kaushik A, Bhansali S, Basu AK. Employing nano-enabled artificial intelligence (AI)-based smart technologies for prediction, screening, and detection of cancer. *Nanoscale* 2024, 16(11), 5458-5486.
  53. Agboklu M, Adrah FA, Agbenyo PM, Nyavor H. From bits to atoms: Machine learning and nanotechnology for cancer therapy. *J. Nanotechnol. Res.* 2024, 6(1), 16-26.
  54. Gao XJ, Ciura K, Ma Y, Mikolajczyk A, Jagiello K, Wan Y, Gao Y, Zheng J, Zhong S, Puzyn T, Gao X. Toward the integration of machine learning and molecular modeling for designing drug delivery nanocarriers. *Adv. Mater.* 2024, 36(45), 2407793.
  55. Singh AV, Rosenkranz D, Ansari MHD, Singh R, Kanase A, Singh SP, Johnston B, Tentschert J, Laux P, Luch A. Artificial intelligence and machine learning empower advanced biomedical material design to toxicity prediction. *Adv. Intell. Syst.* 2020, 2(12), 2000084.
  56. Jahandoost A, Dashti R, Houshmand M, Hosseini SA. Utilizing machine learning and molecular dynamics for enhanced drug delivery in nanoparticle systems. *Sci. Rep.* 2024, 14(1), 26677.
  57. Das S, Mazumdar H, Khondakar KR, Kaushik A. Machine learning integrated graphene oxide-based diagnostics, drug delivery, analytical approaches to empower cancer diagnosis. *Biomed. Mater. Eng.* 2025, 3(1), e12117.
  58. Krishnamoorthy U, Balasubramani S. Intelligent Nanomaterial Image Characterizations—A Comprehensive Review on AI Techniques that Power the Present and Drive the Future of Nanoscience. *Adv. Theory Simul.* 2024, 7(12), 2400479.
  59. Alafeef M, Srivastava I, Pan D. Machine learning for precision breast cancer diagnosis and prediction of the nanoparticle cellular internalization. *ACS Sens.* 2020, 5(6), 1689-1698.
  60. Alalmaie A, Alshahrani HT, Alqahtani M, Alshahrani Z, Alahmari S, Asiri A, Alqadi B, Alshahrani A, Alshahrani S, Akhter MH. Integrating computational insights in gold nanoparticle-mediated drug delivery: enhancing efficacy and precision. *Front. Med. Technol.* 2025, 7, 1528826.
  61. Jia Y, Hou X, Wang Z, Hu X. Machine learning boosts the design and discovery of nanomaterials. *ACS Sustain. Chem. Eng.* 2021, 9(18), 6130-6147.
-

62. Wang J, Liu G, Zhou C, Cui X, Wang W, Wang J, Huang Y, Jiang J, Wang Z, Tang Z, Zhang A. Application of artificial intelligence in cancer diagnosis and tumor nanomedicine. *Nanoscale* 2024, 16(30), 14213-14246.
63. Ali R, Balamurali M, Varamini P. Deep learning-based artificial intelligence to investigate targeted nanoparticles' uptake in TNBC cells. *Int. J. Mol. Sci.* 2022, 23(24), 16070.
64. Szymaszek P, Tyszka-Czochara M, Ortyl J. Application of photoactive compounds in cancer theranostics: review on recent trends from photoactive chemistry to artificial intelligence. *Molecules* 2024, 29(13), 3164.

**How to cite this article:** Fernando Romanholo Ferreira L. The Future Prospect of Integrating Machine Learning and Nanocarbon Materials in Cancer Treatment: A Prospective Review. *Curr. Appl. Sci.*, 2025, 3(2):109-118. <https://doi.org/10.22034/cas.2025.524909.1050>