AI-DRIVEN DRUG DISCOVERY AND PERSONALIZED IMMUNOTHERAPY IN CANCER TREATMENT

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ABSTRACT

AI is revolutionising our understanding of cancer immunotherapy. This aids in identifying drug targets, developing improved treatments, and tailoring patient care accordingly. AI can identify patterns that traditional methods cannot, by analysing big data such as gene expression, single-cell sequencing, and medical scans. By utilising deep learning and associated generative models, researchers can predict drug activity, identify immune system targets, and suggest combinations. Non-invasive imaging and the tracking of tumour response to treatment are made possible by AI. Additionally, while AI still faces hurdles in terms of data availability and ethical considerations, it has the potential to revolutionise cancer care by enhancing efficiency, intelligence, and effectiveness (Olawade et al., 2025; Derraz et al., 2024).

WHY AI MATTERS IN IMMUNOTHERAPY

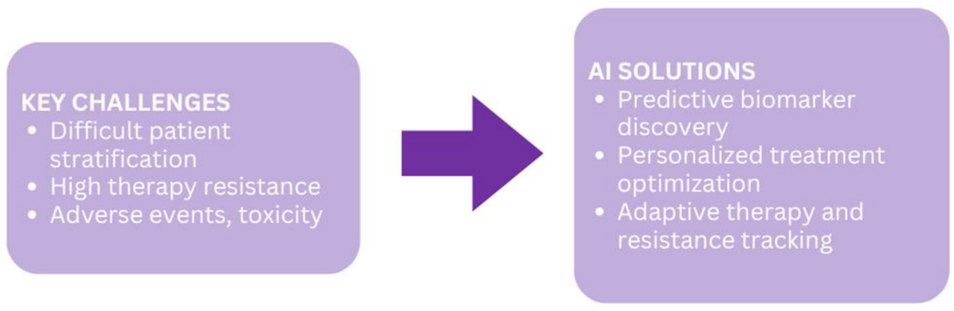

Figure 1: AI tackles key immunotherapy challenges by improving patient selection, reducing resistance, and managing toxicity.

PERSONALIZED IMMUNOTHERAPY

AI enables real-time treatment customization and biomarker discovery.

Key advances include:

- **Novel Resistance Mechanisms Identified**: Explainable AI (XAI) revealed TREM2$^+$ macrophages as key players in resistance to anti-CTLA-4 therapy, leading to the launch of five targeted clinical trials (Derraz et al., 2024).
- **Efficient Biomarker Discovery**: Integrating single-cell RNA sequencing with AI algorithms has reduced the cost of biomarker discovery by 60%, while preserving high accuracy and drastically cutting analysis time (Olawade et al., 2025).
- **Real-Time Treatment Adaptation**: Bayesian network models identified IL-10 upregulation in 73% of CAR-T therapy relapses, allowing for timely therapeutic interventions and improved patient outcomes (Derraz et al., 2024).

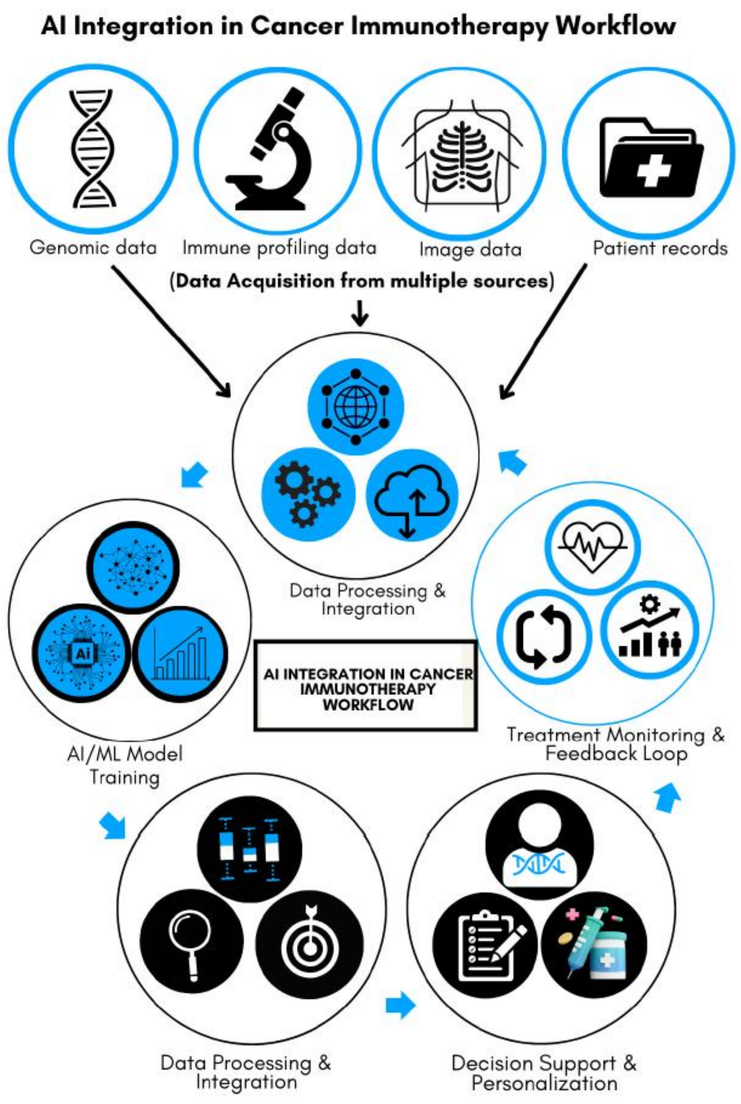

Figure 2: AI integration in cancer immunotherapy workflow (Olawade et al., 2025).

EMERGING TECHNOLOGIES

Radiomics + PET imaging: non-invasive tumor phenotyping (McGale et al., 2024b)
Transcriptomics: ML enhances RNAseq interpretation, splicing, and cell-type mapping (Gui et al., 2023b)
Quantum computing: simulating 1 million immune cell interactions in real-time
Federated learning: data privacy preserved across 47 institutions (CFLI project)

AI IN DRUG DISCOVERY AND DEVELOPMENT

AI drastically reduces drug development time and cost.

Breakthroughs include:

- **Generative AI**: 12,000 neoantigens predicted in 48h, 14% immunogenic (Li et al., 2023)
- **Reinforcement learning**: +47% response in TNBC with optimized ICI + CDK4/6 combos (Prelaj et al., 2024)
- **Graph Neural Networks**: 92% specificity in predicting irAEs (McGale et al., 2024a)

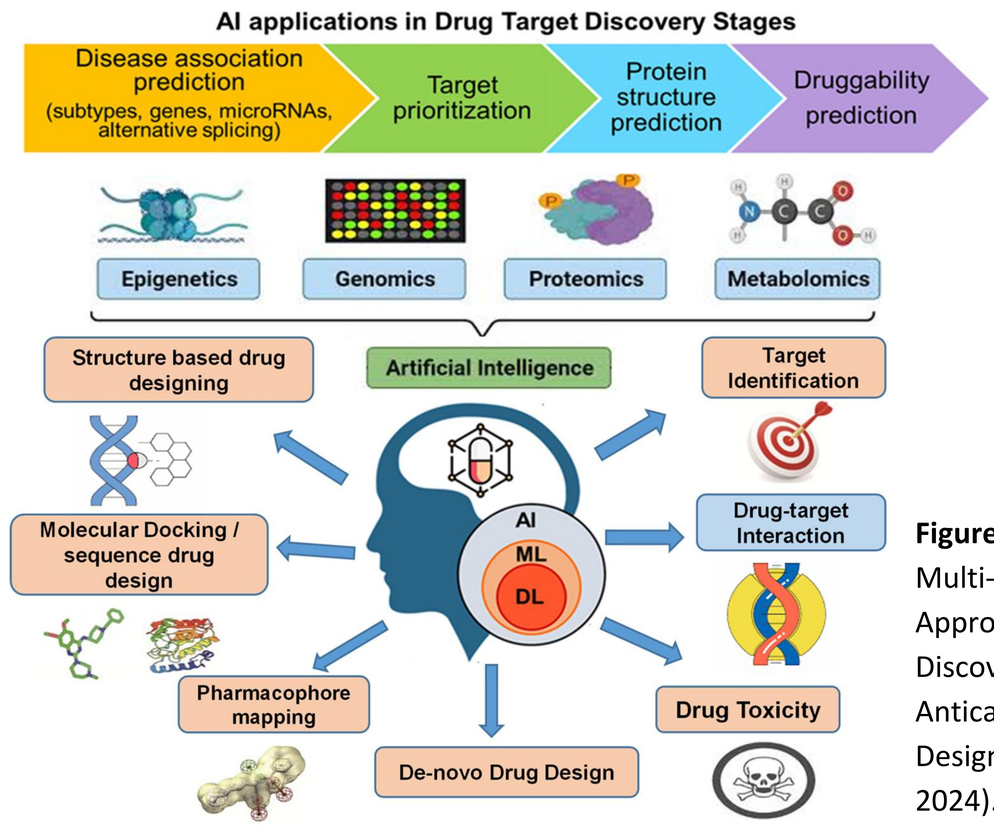

Figure 3: AI-Driven Multi-Omics Approach for Target Discovery and Anticancer Drug Design (Garg et al., 2024).

Applications:

- Target identification from multi-omics (Olawade et al., 2025)
- Binding site prediction for ICIs (PD-1, CTLA-4) (Ogunmola & Aloba, 2025)
- Molecular docking using AlphaFold (Ogunmola & Aloba, 2025)

AI AND TUMOR MICROENVIRONMENT (TME)

Integration of multi-modal data allows AI to understand and reshape the immune landscape.

- Deep learning models predict ICI response with 85% accuracy (Gui et al., 2023a)
- AI-driven TME analysis improved TNBC response from 28% → 41% (Prelaj et al., 2024)
- Liquid biopsy + AI → +32% accuracy in NSCLC survival forecasting (Garg et al., 2024)

CHALLENGES AND ETHICAL CONSIDERATIONS

Despite rapid advances, data heterogeneity remains a major hurdle, with 68% of AI models failing external validation due to batch effects and center-specific protocols (Gui et al., 2023a). Initiatives like ML-SPORE and CFLI promote standardized, privacy-preserving data sharing. Yet, population bias persists—African genomic underrepresentation leads to 2.1-fold higher prediction errors (Derraz et al., 2024). Transparency is key; SHAP analysis is now vital for model interpretability. Regulatory progress lags, with no AI tools yet approved for immunotherapy companion diagnostics. However, quantum simulations of immune responses and adaptive AI-driven trials like DECODE-NIVO signal a transformative future for personalized oncology.

CONCLUSION

Oncology is being revolutionized by the combination of AI and immunotherapy, thanks to three primary mechanisms: accurate formulation of drugs, management of resistance (via dynamic modeling), and discovery of accessible markers. While there are still major issues with data quality, population bias, and regulatory frameworks, AI-powered immunotherapy has shifted from an experimental approach to a clinical necessity.

Synergy may be further developed through the use of federated learning, quantum computing and adaptive clinical trial designs. The end goal is not to replace clinician judgment with AI, but to provide the necessary tools for creating effective cancer treatments that are personalized and successful.

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This research was supported by the Slovenian Research and Innovation Agency (ARIS) through the Core Finding no. ***P1-0045****.*