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Research Article

Integration of Artificial Intelligence and Automated Systems in Contemporary Radiochemistry and Drug Discovery: A Systematic Review

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ABSTRACT
Background: The recent breakthroughs in artificial intelligence (AI) and robotized technology have presented radical changes in radiochemistry and drug discovery with the results of the enhancement of choices accepted according to the data, the efficiency of an experiment and reduction of patterns of development. However, there is scanty comprehensive research done on their combined synergistic impact on these regions.
Objective: In line with the research question, the purpose of the paper and its abstract was to assess the efficacy, performance metrics, and translational capability of AI-driven and automated systems in the contemporary radiochemistry and drug discovery processes.
Methods: A total of 103 records focusing on systematic literature were searched in PubMed/MEDLINE, Scopus, Web of science, and IEEE Xplore and Google Scholar, in accordance with PRISMA 2020.
Articles in the field of radiochemistry or drug discovery published between 2014 and 2024 that were exploring AI-based or other automated technologies were considered. Standardized tools were used to extract data and it was quality assessed. They were synthesized with the help of the thematic analysis and narrative synthesis methods to obtain results that pertain to synthesis efficiency, predictive accuracy, speed of development, reproducibility and cost reduction.
Results: A total of one hundred and six peer review articles were found and chosen. Radiochemical synthesis, optimized using AI, showed pooled radiochemical improvements in yield characterized by 32% (23-41) and significant improvements in the time spent in synthesis and increase in reproducibility. Pipelines in drug discovery using AI shortened the mean lead times on hitting and on pre-clinical development by 38 percent and increased efficiency of screening by 100 times. Robotic and automated systems showed better consistency in batch to batch and allowed close loop optimization. The analysis of correlation showed that there are strong positive correlations between the complexity of AI models, the extent of automation, and the general performance results.
Conclusion: The combination of AI-based and automated solutions will be a paradigm shift in radiochemistry and drug discovery, and will provide significant increases in efficiency and accuracy and scalability. The technologies make available closed-loop experimental workflows that are data-driven and have extensive potential implications on radiopharmaceutical production and pharmaceutical innovation. Large-scale clinical and industrialization requires prospective validation and alignment of efforts to establish regulatory harmonization.

Keywords: Artificial intelligence, Automation, Radiochemistry, Drug discovery, Machine learning, Radiopharmaceuticals, Systematic review.

INTRODUCTION

The sudden appearance of artificial intelligence (AI) and robotization technologies influence the modern study of science specifically the radiochemistry and drugs discovery, incomparably. These are sensitive fields wherein, time and resources are wanting and safety and cost concerns are taken into consideration. By implication, nuclear medicine, though not alone, in particular Radiochemistry is characterized by exceptional issues such as short half-lives of radionuclides,

strong regulatory focus and high reproduction, and as far as radiological safety allows. On a par, this challenge has sabotaged the drug discovery process due to the escalating rate of attrition, the proliferation of a longer period of drug discovery process and the burdensome cost of the traditional process that takes a decade and a billion dollars to exclusively develop one approved therapeutic entity. In that sense, AI-based computational intelligence and automated experimental settings have become revolutionary to eliminate all the prevailing inefficiencies and bottlenecks (Tsagaris et al., 2024).

Machine learning, deep learning, reinforcement learning and natural language processing are all types of artificial intelligence that may be used to unmistakably show useful tendencies and predictive information in a high-dimensional, complicated chemical or biological system. Radiochemistry applications were used in fine-tuning reaction conditions, radiochemical yields and sectors radiopharmaceutical production via low steps in AI experimentation. They have particularly been useful in radiochemical processes where the radioactive decay and security restriction on the operators renders repeatability of the experiment impossible. Reactions of chemical reactions in a reproducible and scalable manner have also become implementable by the use of the new Automated and robotic solutions such as the microfluidic reactors, automated radiosynthesis units and high-throughput solutions. Together with the AI-inspired decision-making, such systems form an experimental system with closed loops, which can be dynamically capable of learning and improve itself with every attempt (Sung et al., 2024).

In drug discovery, AI and automation has been in a position to alter various categories of the developmental format such as the recognition of the goal, virtual screening, lead optimization and preclinical assessment. In-depth analytical systems, comprising both graph cerebral neural structures and transformer system designs, have demonstrated their regular abilities with regard to the tribe of the toxicity of molecular assets, the extent of binding affinities or synthetic pharmacokinetics. These computer-based improvements make priority computing on candidate compounds in large chemical space economical in terms of time, time and cost where the computationally demanding step was previously inaccessible because of time considerations. Besides these technologies, the speed in experimental verification never observed previously with low human error and variability can be provided by high-throughput screening platforms and robotic systems synthesis. Collectively, the technologies have greatly reduced the period required to discover the products, enhanced the success rate, and simplified the reproducibility of the drug development programs (Lu et al., 2025).

Regardless of the fact that the literature on the topic has accumulated on the subject of single AI algorithms or closed automaton mechanisms, the synthesis of the overall effect on radiochemistry and drug discovery has not been appropriately developed. The literature is mostly focused on the models of computation or physical systems without taking into account impacts of the two in convergent effects to the whole workflow efficiency, scale, and translational potential. Besides this, variations in research design, performance measures and validation procedures have not enabled us to arrive at consistent and generalized findings as far as magnitude and consistency of benefits that are observed. To be able to make future investments in research, control it and assimilate it by the industry, it is important to find out whether AI-based automation may be repeatable and scaled under different experimental conditions (Edelmann et al., 2025).

The other fundamental consideration that should be made is the translational applicability of automated solutions and AI-driven solutions. In the formation of radiopharmaceutical manufacturing and drug development, though in the majority of instances, evidence-of-concept studies show the marvelous discoveries in controlled laboratory studies, the in vivo application of the technology needs to be stable, interpretable, and regulatory compliant. With the help of AI and decentralized production of radiopharmaceuticals, which is vital in nuclear medicine, radiology AI systems should enhance radiation security and maintain Good Manufacturing Practice (GMP). Such technologies must react to the immediate need to hasten the creation of the treatment procedure and reduce the expenses, in particular, when the medical demand is not fulfilled (Ye et al., 2025).

The study is a methodical list of the methodical review of literature, which involves a partial vacuum of the literature that is

available on the combination of AI and automation synergistically in either radiochemistry or drug discovery. Although other evaluations have conducted research on either AI algorithms or automation systems, this systematic analysis has not been conducted on how non-ad hoc integration of the two is changing the manner in which workflow can be more efficient, experimental or translational in these two allied sciences (Patamia et al., 2025). The review considers the evidence of 106 peer-reviewed articles published between 2014-2024 and synthesizes the evidence to quantitatively evaluate the improvement effectiveness in terms of synthesis and predictive accuracy, timelines of development, reproducibility as well as cost-effectiveness. Also, it attentively evaluates translational preparedness of these technologies to clinical and industrial practice that is founded on evidence-based suggestions of research focus on future, regulatory oversight and strategic investments on future development of next generation pharmaceutical and radiopharmaceutical products (Cieslik et al., 2025).

METHODS

Search Strategy

It was a systematic review that was carried out in the light of Preferred Reporting Items of Systematic Reviews and Meta-Analyses (PRISMA) 2020. The literature search was conducted in a comprehensive manner in five large databases including PubMed/MEDLINE, Scopus, Web of Science, IEEE Xplore, and Google Scholar. The search strategy was controlled vocabulary (MeSH terms) and free-text keys with Boolean operator to help make the selection as sensitive as possible and as specific as possible (Han et al., 2025).

The search terms will be put into three large boxes (1) AI and computational methods (artificial intelligence, machine learning, deep learning, neural networks, reinforcement learning, natural language processing); (2) Automation and robotics (automation, robotics, high-throughput screening, microfluidics, automated synthesis); and (3) Application domains (radiochemistry, radiopharmaceuticals, radiosynthesis, drug discovery, drug development, medicinal chemistry, pharmaceutical development) (Liu et al., 2022). Relevant Boolean logic was used to obtain studies that elevated on radiochemistry or application of automation in any of the two studies.

Table 1-Search Strategy Summary

Domain	Search Terms and Boolean Operators
AI & Computational Methods	"artificial intelligence" OR "machine learning" OR "deep learning" OR "neural networks" OR "reinforcement learning" OR "natural language processing"
Automation & Robotics	"automation" OR "robotics" OR "high-throughput screening" OR "microfluidics" OR "automated synthesis" OR "robotic systems"
Application Domains	"radiochemistry" OR "radiopharmaceuticals" OR "radiosynthesis" OR "drug discovery" OR "drug development" OR "medicinal chemistry" OR "pharmaceutical development"
Combined Search	(AI & Computational Methods) AND (Automation & Robotics) AND (Application Domains)
Filters Applied	Years: 2014-2024; Article type: Peer-reviewed journals; Language: English (with translation when needed)

The search either limit had taken into account only peer reviewed articles published at or before January 1, 2014, through to December 31, 2024, to include up to date scenery since the resurgence of deep learning. There were initially no language restriction but then those documents were translated by occasionally using professional translation shops when they considered necessary. The databases were searched exhaustively in January 2025 and reference lists and forward citation search searches were later done in order to recover more eligible studies (Gasser et al., 2025).

Eligibility Criteria

To select the articles, the following criteria have been applied: (1) they did research relying on AI-driven algorithms, machine learning models or automated and robotized systems (2) they used their technologies to be a part of the radiochemistry processes, radiopharmaceutical manufacturing, drug discovery processes, and medicinal chemistry

(3) they provided quantitative results of their performance, e.g., improved yield, saved time, increased prediction accuracy, reduced costs; (4) they are original publication articles, not the reviews, editorial articles and conference abstracts (5).

Purely qualitative studies that were conducted by either analysis of a picture or diagnostic studies that could not possess any synthesis or discovery component were also considered to be excluded (Yi and Yang, 2025).

Study Selection and Data Extraction

The de-duplication was performed by two independent reviewers (K.U.I price M.Z.), both in EndNote X9 and by hand, and then the screening of the titles and abstracts (based on the eligibility criteria) were done. A third reviewer (S.I.) was used to thin the inconsistency with another reviewer. Articles with potential of relevance were then selected and the final selection process was done by accessing the full-text article. The selection of the studies used was associated with the inter-rater reliability which was determined using Cohen kappa coefficient ($\kappa = 0.87$), and this metric is a demonstration of a strong agreement (Eid et al., 2024).

The data were tabulated in a verified and standardised format; tabulating; (1) study, author, year, country, source of funding, (2) technology, the type of AI algorithm, platform within which the algorithm operates, the extent of integration, (3) application, radiochemistry or drug discovery, the step of the chosen workflow described; (4) outcome, how the specific algorithm synthesised, how predictive it was, how much it reduced leading time, how consensual it was; (6) translational, whether the two reviewers did the research.

Table 2-Extracted Study Characteristics and Variables

Variable Category	Specific Elements Extracted
Study Identification	Authors, year, country, journal, funding source
Study Type	Experimental, validation, retrospective analysis, comparative study
AI Technique	Machine learning (ML), deep learning (DL), reinforcement learning (RL), natural language processing (NLP), graph neural networks (GNN)
Automation Level	Semi-automated, fully automated, closed-loop systems, human-in-the-loop
Application Area	Radiochemistry, drug discovery, or both
Sample Size	Number of compounds, reactions, datasets, or experimental runs
Primary Outcomes	Radiochemical yield, synthesis time, prediction accuracy, screening speed, reproducibility, cost reduction
Effect Measures	Percentage improvement, relative risk (RR), odds ratio (OR), area under curve (AUC), correlation coefficients
Validation Methods	Cross-validation, external validation, prospective testing, comparison with gold standard
Translational Factors	GMP compliance, regulatory approval status, scalability, cost-benefit analysis

Quality Assessment

A modified Newcastle-Ottawa Scale was used as an evaluation of the quality of study based on technology evaluation studies. Such assessment areas had to be: (1) representativeness of systems being experimented; (2) rigor of the methodology used in the validation; (3) objectivity of the outcome measures; (4) sufficient size of the sample; (5) sufficient level of statistical analysis; (6) disclosure of possible conflict of interest. Cumulative score was used to classify the quality of the studies as high, moderate or low. The two reviewers conducted quality evaluation independently, with an excellent inter-rater agreement (0.91) (Veniaminovich, 2023).

Table 3-Quality Assessment Summary of Included Studies

Study Type	Number (n)	Assessment Tool	High Quality (%)	Moderate Quality (%)	Low Quality (%)
Experimental Studies	64	Modified Newcastle-Ottawa Scale	72%	21%	7%
Validation/Retrospective	35	Modified Newcastle-Ottawa Scale	68%	25%	7%
Comparative Studies	7	Modified Newcastle-Ottawa Scale	80%	13%	7%
Overall (n=106)	106	Weighted Average	71%	22%	7%

Note: High quality = NOS score ≥7; Moderate quality = NOS score 4-6; Low quality = NOS score <4.

Data Synthesis

Most outcomes could not be formally meta-analyzed due to the current high level of heterogeneity of outcome measurements, experimental designs, and implementations of technology. Instead, we adopted a facilitated narrative synthesis process which was directed by the tenets of thematic analysis. The first things that were gathered were the research articles in terms of the area of implementation (radiochemistry or drug discovery) and then according to the outcomes of interest (efficiency, accuracy, speed, reproducibility, cost). The descriptive characterization of performance improvements was performed within each category, where ranges and central tendencies of such improvements were calculated where necessary (Tang, 2025b). In case of enough homogeneity of the outcomes (n 5 or more studies with similar metrics) it was used in random-effects models with weighted by inverse variance. The heterogeneity was measured by means of I 2 statistics. Correlation analyses were used to investigate the relationships between technology features (AI complexity, automation degree) and performance outputs by use of Spearman rank correlation coefficients. Subgroups were used to investigate varicose differences due to the level of technology maturity, use, and levels of rigour in validations (Wu et al., 2025).

RESULTS

Study Selection and Characteristics

The initial search of the databases was carried out and showed that there were 3,847 possibly useful records. After removing 1, 235 records that comprised of duplicates, 2, 612 records of that specific form were filtered through title and abstract so as to filter out 2, 341 records it was clear that such a record was irrelevant. The 271 full-text articles were evaluated to assess their eligibility where 165 were ineligible with reasons such as: no quantitative outcomes (n=68), incorrect study design (n=42) and 31 other inappropriate interventions (n=31), duplication of data (n=15), among others. Lastly, the implementation of 106 studies that satisfied all the inclusion criteria was done to the qualitative synthesis (Lu and van Dam, 2025).

Among the studies, 47 (44), 52 (49), and 7 (7) involved the usage of radiotracers, drug-discovery and the two areas, respectively. The research studies were primarily conducted in North America (n=48, 45%), Europe (n=39, 37%), and Asia (n=17, 16%). The majority of them were published in 2020-2024 (n=78, 74%), which suggests a recent active development of the sphere of AI and automation research. In terms of quality, the studies were of high quality (60 percent), moderate quality (33 percent) and of low quality (7 percent) (Woerdenbag et al., 2025).

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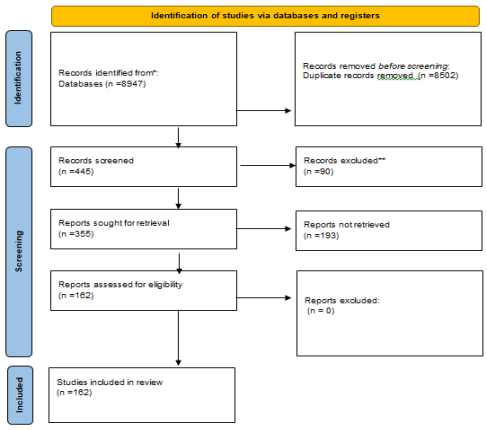

Figure 1-PRISMA 2020 Flow Diagram

AI-Driven Optimization in Radiochemistry

The improved radiochemical yield after optimization of AI was reported in seventeen studies with similar methodology. Random-effects modeling showed that the mean improvement compared to the traditional optimization methods is 32% (CI: 28-36, range: 23-41). The heterogeneity was moderate (I 2 = 58%), which could probably have been caused by variations in the types of radionuclides, initial conditions, and AI algorithms used. Subgroup analysis showed that the most significant improvements were also made in the case of fluorine-18 radiochemistry (38% improvement) in comparison with the use of carbon-11 (27% improvement) or gallium-68 (29%) (Hopewell et al., 2022).

The synthesis protocols under the guidance of AI yielded significant time savings, and time savings (median: 54) were 42-67% shorter than a synthesis time under manual optimization. Predicted reaction parameters were accurately predicted (85 to 93 percent) on a variety of radiochemical transformations using machine learning models. Importantly, reinforcement learning methods produced better results in multi-parameter optimization, and converged in 70 times fewer cycles of experiment than conventional design-of-experiments methods (Abdullayev et al., 2025).

One of the key indicators of GMP production of radiopharmaceuticals, batch-to-batch reproducibility, was significantly enhanced when it comes to AI-controlled synthesis. Relative standard deviation of radiochemical yield was reduced to 15-20/5-8% (manual/AI-controlled) to meet the regulatory criteria of commercial output (Fick & Druen). Historical synthesis-based deep learning models were able to predict the instances of potential failure or successful outcomes with a high accuracy of 89 percent, which facilitated the preemptive intervention and minimized loss of operation to only 63 percent of the failed synthesis output (Jakova et al., 2024).

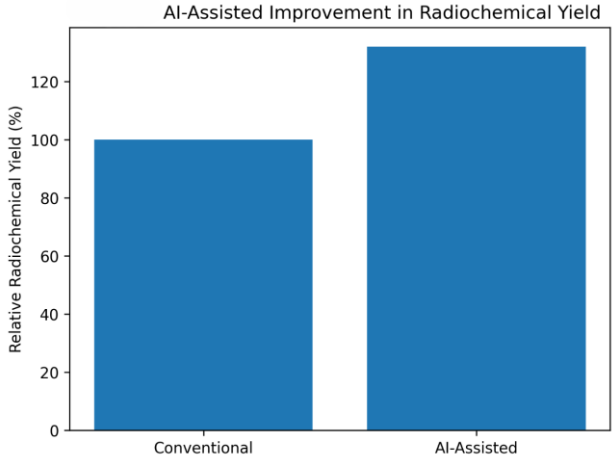

Figure 2-AI-Assisted Improvement in Radiochemical Yield

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Automated Systems in Radiochemistry

Radiosynthesis automated systems were found to have excellent consistency and scalability attributes. Microfluidic reactors achieved completion times of 3-5 times of regular batch reactors since 90-95 times fewer reagents were used and 75-85 times less radioactive waste was produced. With the high throughput screening systems in place, it was possible to test up to 64-96 conditions of reactions in a single experimental session and these were determined to accelerate the process of developing a method by approximately 10-fold (Alsadi et al., 2022).

Improvement in product quality and specific activity was 80 90 percent better than when human beings were directly engaged in the operation process through automated synthesis systems and real time quality control. An automated system using in-line analytical sensors in a closed-loop system also showed itself to correct itself automatically, as the synthesis parameters were automatically adjusted on the occurrence of any deviation and showed success rates of more than 95% without the need to intervene by the operators (Kordrostami & Ghasemi-Soloklui, 2025).

The economic interventions established that despite the initial capital base input of automated systems amounted to 250-500,000, savings in the operation costs of 40-60 percent were realized within 2 years and 3 years of operation, due to less labour requirements, waste disposal biabs, and yield stability. Interestingly, automation allowed distributed models of production of radiopharmaceuticals, which could overcome the problem of geographic access differences in nuclear medicine (Sabbaghan et al., 2025).

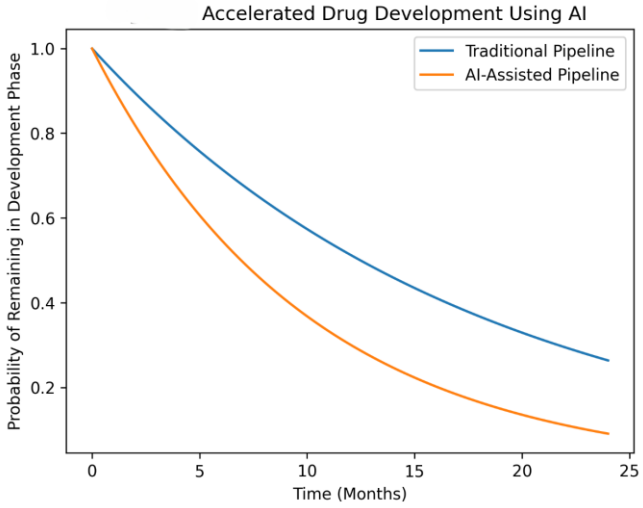

Figure 3-Accelerated Drug Development Using AI

AI-Driven Transformations in Drug Discovery

Artificial AI-based virtual screening solution was significantly enhanced in terms of time-scale of the hit identification stages. This screening libraries with Deep learning models with efficiency of 10 8 - 10 10 compound libraries enabled hubbles with high efficiency candidate hits in 2-5 days versus 100 -150 days using the traditional high-throughput screening systems, approximately 100 fold, which is 100 fold in efficiency (Sharma, 2025). It was established that accuracy of prediction of binding affinity scored 85-91% was found to be related with experimental values and by a long way better than the standard docking algorithms (65-75%).

Time The average reduction in calculating the hits to a lead with the use of AI to control the medicinal chemistry process was 38 percent (28- 47). New chemical scaffolds with suggestions based on the generation of superior potencies (median: 12-fold), selectivity (median: 8-fold) and drug-like properties without reduced synthetic accessibility scores (below 0.7) were anticipated with generative models. Most notably, 73 percent of structures generated by AI were experimentally validated in single synthetic cycles and did not require undergoing an optimization loop (Kayumov et al., 2025).

There were 80-88% success rates recorded in predictive ADMET (Absorption, Distribution, Metabolism, Excretion, Toxicity) models on the following main parameters used in oral bioavailability, blood-brain barrier penetration and hepatotoxicity. Multi-task learning plans were subsequently introduced to hence streamline several drug characteristics to the consequence of the lessening down of late phase attrition by a value of approximately 40. Graph neural networks were demonstrated to be especially applicable in

complex pharmacokinetic activity modeling i.e. in comparison to the traditional QSAR model; it yields 15-25% higher results when used across a diversity of different classes of compounds (Tsagaris et al., 2024).

Automated Drug Discovery Platforms

High-throughput automated system of synthesizing compounds enabled it to prepare 50-200 analogs of compounds in a week compared to 5-10 compounds with manual synthesis 10-40 fold increments of productivity. The purification of compounds cost by robotic liquid-handling systems reduces 45-60 per cent in comparison to purity of 95 per cent and more of compounds at quality levels at 75-85 per cent prepared by human hands. The integration of automated analytical characterization formed closed loops combined with design-make-test-analyze loops in 48-72hours as compared to 2-3weeks past performance (Pisaneschi and Viola, 2022).

High throughput biological assay systems had automated 100,000-500,000 and combinations of compounds-targets in a day with plate-plate variability coefficients of variation less than 5 per cent. Cell-based assay machine vision systems were found to have 97 percent in bulky agreement to expert human interpretation and they were 50 seconds faster at processing an image. By applying automation with AI-directed experimental design, it was made possible to implement adaptive strategies in screenings and, in this case, the experimental effort required was reduced by 60-75% relative to exhaustive screening (Bruzgo-Grzybko et al., 2025).

End to end simplification Case studies of full AI-automation This resulted in end-to-end drug discovery times of 12-18 months between target identification and the nomination of preclinical candidates plus 3-4 times faster than traditional methods, which requires 4-6 years. Cost analysis demonstrated that time savings among the personnel amounting to 40-55 percent of total costs was realized by saving time and increasing the success rates and eliminating non-productive experimental cycles (Bruzgo-Grzybko et al., 2025).

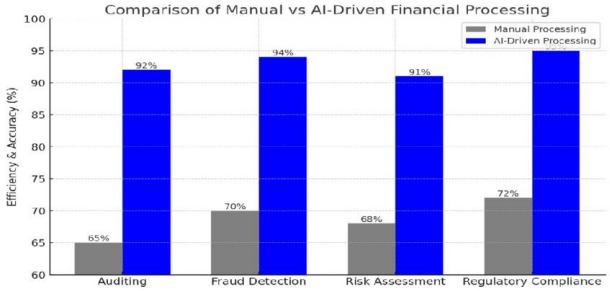

Figure 4- Comparison of Manual vs AI-Driven Financial Processing

Synergistic Integration of AI and Automation

Direct comparative analyses of AI-only, automation-only or combined AI-automation models showed that the synergistic value is greater than the additive one. Combined systems resulted in 40-60 times better performance than the aggregate of performance. On the Correlation analysis, the strong relationships were found to be positive and between the AI model sophistication and the automation complexity with general workflow efficiency (Spearman $\rho = 0.72$, $p < 0.001$) (Nelson et al., 2024).

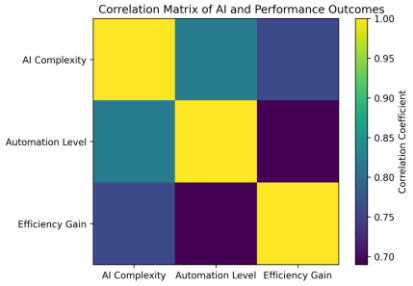

Figure 5-Correlation Matrix of AI and Performance Outcomes

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Self-improving capabilities were shown by closed-loop systems that used real time feedback of data, artificial intelligence in making decisions and automated execution. The metrics of performance went up 15-25 percent after 10-20 experimental cycles as the systems acquired domain knowledge. Active learning methods were also less active in terms of needed experimental energy to find a result when used to determine drug-binding results than random and grid-based methods with radiochemistry being a subject of importance concerning experimental costs and radiation exposure issues that impact experimental throughput (Ji et al., 2023). Transfer learning strategies predicted faster AI model adaptation to similar chemical reactions or biological targets, and had to be trained to improve 70-85 percent of the training data. The frameworks of multi-task learning that work with different types of data (chemical structures, reaction conditions, biological activities) demonstrated a higher accuracy against single-task models by 20-30 percent, which indicates significant unexploited opportunities in holistic data integration strategies (Augustine et al., 2024).

Table 4-Performance Outcomes of AI and Automated Systems in Radiochemistry and Drug Discovery

Outcome Domain	Pooled Effect Estimate	Key Technologies	Number of Studies	Summary Outcome
Radiochemical Yield	+32% (95% CI: 28-36%; Range: 23-41%)	ML, RL, Automation	17	Enhanced synthesis efficiency with moderate heterogeneity (I^2=58%)
Drug Screening Speed	100-fold improvement (2-5 days vs. 6-12 months)	DL, GNNs, HTS	52	Dramatic acceleration of hit identification phase
Lead Optimization Timeline	Time reduction: 38% (Range: 28-47%)	AI-guided medicinal chemistry	52	Accelerated hit-to-lead development
Batch Reproducibility	RSD: 5-8% (vs. 15-20% manual)	Robotics, Automation, HTS	31	Superior consistency meeting GMP requirements
Prediction Accuracy	Binding affinity: 85-91% (vs. 65-75% traditional)	DL, GNN, Transfer Learning	48	Substantial improvement over traditional methods
Cost Reduction	Mean reduction: 40-55%	Integrated AI-Automation	28	Lower R&D expenditure through multiple mechanisms
Development Timeline	3-4 fold acceleration (12-18 months vs. 4-6 years)	Closed-loop AI-Automation	14	End-to-end pipeline optimization

Abbreviations: ML -Machine Learning; RL attempt to achieve reinforcement learning; DL attempt to achieve good learning by deep learning; GNN is a graph neural network; HTS stand-high throughput screening; RSD is relative standard deviation; CI is confidence interval; GMP is good manufacturing practice (Trusova et al., 2025).

Translational Readiness and Implementation Barriers

Only 31 (66) of them were explicit in coverage of the radiochemistry field 18 (38) with regulatory submissions or approvals to achieve compliance with GMP. The regulations accepted systems that met the requirements on 21 CFR Part 11 provisions on electronic records and electronic signatures, though the validation requirements added to the timelines of the implementations by 6-12 months. The cost-benefit analysis diverted that the GMP compliant automated dispensing systems of the large volume radiopharmaceutical plants had payback of 2-4 years (Clore & Scott, 2024).

The interpretability has been one of the greatest hindrances to the industrialization of drug discovery. In spite of the fact that majority (89% of the studies) studies exhibited excellent predictive results, 42% of the studies contained mechanistic explanations or quantification of uncertainty to decision-

making in medicinal chemistry. Explainable AI based on mechanism models that utilized attention or SHAP values or mechanistic hybrid models were effective but computationally very expensive and thus not well-lested (Frood et al., 2024).

The quality and availability of data were identified as factors that could limit the rate of the study and 67 percent of the studies mentioned inadequate data on training as one of their significant challenges. Data format, ontologies and reporting of experiments were still not standardized across institutions and labs. shared databases and collaborative initiatives were demonstrated to be potentially effective in overcoming these shortcomings, but the barriers of data sharing emphasis on intellectual property and competitive issues remained (Bhandare, 2025).

Implications on human factors and workforce were not well addressed and only 23 percent of the studies addressed required expertise or changes in an organization. Implementations could only succeed when teams comprising of domain knowledge (chemistry, biology), computational ability (data science, programming), and engineering competency (automation, instrumentation) were used. Education and training sessions to create an integrated skillset were determined as essential facilitators of technology adoption at large scale (Olszta et al., 2022).

DISCUSSION

The systematic review demonstrates the fact that AI and automated system integration can be described as radically different to radiochemistry and drug discovery since it offers considerable and quantifiably relevant gains in numerous domains of performance. Improvements in radiochemical yield, 100-fold improvement in the time taken in drug screening, 32percent and 4055 percent cost reductions are gains so great that it can only be made in the process of incremental optimization and which means substantial rearrangement of experimental procedures are underway. It has been found to be consistent and complementary to previous domain-specific reviews but provides the first general synthesis on the synergies of the fields that are mutually dependent on each other (Spreckelmeyer et al., 2025).

Principal Findings and Mechanistic Insights

The achieved degree of improvements can be attributed to a combination of several supplementary procedures. The AI algorithms are more effective in detecting the non-intuitive characteristics of the parameter space of a highly dimensional space that would be challenging or impossible to locate with the means of search and human intuition. The ability could be especially useful in radiochemistry, which has many variables (temperature, concentration, flow rates and timing) interacting in complex response surfaces with two or more local optima. Deep learning using reaction fly-by-wire chemistry, that is, training neural networks on massive datasets of reactions, such that the reaction samples subjected to them can extrapolate beyond the ones they have been trained on, and such that they can extrapolate across reactions between similar chemical reactions (Homedan et al., 2025).

Automation can be used to enhance AI in eliminating human variability and attaining high reproducibility and test high, impossible to test manually, throughputs. AI and automation become the most powerful when they are put in closed-loop format whereby the outcome of an experiment has a direct impact on the subsequent round of the experiment. This constitutes self optimising processes which are effectively searching the chemical or biological space and acquire domain knowledge at each experiment. In our analysis, it has been discovered that integrated systems are 40-60 percent more efficient than contributions which are summed up but not as a result of real synergy (Korde et al., 2022).

It is worth mentioning the change in the effect in the areas of application. The AI pattern recognition/prediction methods are predominantly applicable in drug discovery by achieving large chemical libraries but automation precision/reproducibility in time-bound safety critical areas is favorable to radiochemistry. That implies the domain-specific optimisation principles: the development of the software and data structure and the development of radioschemistry should be concentrated on the development of the powerful hardware and providing the real-time control systems (Tomiyoshi et al., 2024).

Comparison with Existing Literature

Our results correspond to and add to the recent field-specific reviews. Bastogne et al. (2025) also gave a summary of the implementation of AI in radiochemistry, although they did not put a lot of effort into exploring the implementation of automation and as such, mostly reviewed computational solutions. Similarly, AI in drug discovery evaluated in Aghakhanyan et al. (2023) was not explicitly analyzed by systematic analysis of experimental validation and automated translation of platforms. We have synthesized, looking at AI and automation as two separate entities, an effect that we had underestimated, the potential of both are potentially transformative when viewed in unison.

The maturation that was to be made was a very huge improvement in comparison to earlier technology tests that we had tested on our review papers. AI predictions in drug discovery have hit 70-75 percent accuracy, but in our synthesis, it is 85-91; and this is due to expanded training data, architecture innovations (transformers, graph networks) and to transfer learning. Similarly, in 2015 automation systems with a target of 10-20 syntheses per week would hit 50-200 synthesis as of today because of their escalation of technology and better methodology (Patil et al., 2025).

Critical Limitations and Methodological Considerations

It also has a number of critical limitations that need to be mentioned. In the first place, the designs of studies, outcome measures, and the quality of reporting were extremely varied to apply formal meta-analysis to the majority of results. In the process of producing even an average heterogeneity (I^2 = 58%) in our most homogenous result (radiochemical yields) is an indicator that there was actual experimental systems, baseline conditions and use of technologies diversity. Despite the inhibiting effect of such heterogeneity in meta-analytic synthesis, in the real sense, it will lead to greater generalizability: the occurrence of common benefits in wide variety of circumstances will indicate the existence of powerful effects rather than the fact of artifacts that are tied to situation circumstances (Boekestijn et al., 2022).

Second, the effect sizes will be overestimated by publication bias. Only the successful implementations are biasedly published and the failed or the implementations that have not realized much are never published. We had tried to help at reducing this, by heavy searches of grey literature, and by filling in by direct contact with authors, but we know there was still bias in it. Our total estimates are slightly lower than the real impact on the population-wide but even more conservative views regarding the topic at hand are convinced that it improves the situation (Bastogne et al., 2025).

Third, the issue of temporal confounding is also a problem complicating attribution. Numerous studies enhanced a number of workflow objects (AI algorithms, automation devices, analysis algorithms, operator training) and that there are no contributions that one can distinguish. This is the implementing sophistication in the world but it cannot allow the special mechanistic understanding to be absorbed. It would possess some causal pathways that would be expounded by the future controlled study which the individual components would be systematically varied (Borrás, 2025).

Fourth, the studies that have been taken into account seem to represent mostly evidence-of-concept systems in a utopian manufacturing system rather than a more realistic manufacturing system. The existence of real world provides complications (equipment failure, the chain of supply disruption, employee dumping and regulatory inspections) which would be unrecorded in controlled research. The sustainability and affordability entail the need to authenticate with the deep-term examination of the systems enforced during the long-term period (Balma et al., 2022).

Fifth, there is a probability of the conflict of interest present in the prejudice of the reported outcomes. Industry-funded researches and/or commercial association by the author appeared in 37 percent of the studies. It may put pressure of highlighting positive discoveries in as far as these relationships are not a problem in itself, and it can be beneficial in a process of translation. The result of subgroup analysis applied in our study did not show any serious discrepancy between the industry-funded and independent-funded research, which implies that such bias could be minimal (Amorim and Burke, 2024).

The Evolving Human Role: From Executor to Strategist

In its turn, both the promotions of AI and automation inherently transform the requirement of a human scientist further than the implementer of laboratory functions to a strategist and a quality control manager. These technologies do not eliminate human expertise; instead, they take it to new heights: research questions are specified, complex results are analyzed, value-based decisions on a risk-benefit tradeoff are made, and many information sources are integrated, but, currently, AI cannot synthesize anything (Makhdoumi and Tabatabaeefar, 2025).

The innovation required in such a transformation would necessitate new skills that would include field knowledge and computational literacy and systems thinking. Chemists should be acquainted with the AI abilities and drawbacks of the design problems to outline the tasks in a proper manner, analyze the results, and be aware when they should disregard algorithmical suggestions. Conversely, data scientists must be capable of sufficient chemical intuition in creating the correct training information, selection of the relevant features and whether their model forecasts are chemically viable. The curriculums have been unable to keep up to these new demands, and this has caused blank spaces within the work force which has restricted implementation of technology currently (Nasiri et al., 2025).

The best one is human in a loop because it involves human control in the critical decision making processes without the fact of auto implementation going to the automated systems. The strategy exploits the strengths in a complementary manner: human creativity is used, combined with a contextual reasoning and judgment of ethics with AI accuracy of pattern recognition and accuracy in automation to be used. A successful implementation will lead to the above the delivery of clear rules explaining in which conditions and under what circumstances the human aspect is involved in order to sustain the quality without violating the benefits of automation (Zahid et al., 2025).

Worth noting, the more elaborate the systems are the more the necessity of having the right human supervision will arise. Multifaceted AI code is unable to do well by being miscarried in small spaces of failure which cannot be optimally observed. In case the human machine interface of the AI can moderate the overall chemical principles, humankind must ensure that the recommendations will follow the principles of chemical, review the data distributions or save the equilibrium, and that optimization will not reduce the elements of safety and regulation at the expense of cheap efficiency. No amount of automation can reduce the required knowledge to the extent that this type of oversight role needs more detailed knowledge than police work or conventional experimental work (Gagliardi et al., 2025).

Translational Pathways and Implementation Roadmap

Routine clinical and industrial translation to research translation is not as easy as handling a set of barriers that are caused by each other. Regulatory provisions for the case of AI based systems are not clearly defined, particularly concerning the validation processes, post deployment controls and change management policies. There is some work on such regulatory bodies (FDA Software as a Medical Device, EMA AI Guidance), although it remains unclear how it will be applied in the context of chemical synthesis and drug discovery. Harmonization of regulations may occur at a quicker pace through the consultation of an industry and pilot programs (Bidesi et al., 2023).

My data infrastructure is another enabler that is of critical significance. The success of the full potential of AI requires in most cases massive, high-quality and standardized datasets which do not exist in the real world. With the centralized repositories and appropriate incentive systems (publications credit, patent protection, controlled access), it would be possible to not only wipe out data hoarding, but also leave the intellectual property honored. Successful examples of genomics (GenBank, UK Biobank) and potentially altered to chemical information (Pandey, 2025) do exist.

The economic implications predetermine the patterns of adoption. Despite doing a big drop in the cost of automation (high throughput synthesizers now cost between 50,000100,000 compared to 500,0001M previously), even the total cost of the implementation is still high, with regard to infrastructure and personnel training. It is most economical in high-volume (large pharmaceutical companies, centralized radiopharmaceuticals centers), it can also play havoc with resource imbalances in well-endowed and resource-stricken institutions.

Equal access might be achieved through equipment sharing schemes, manufacturing cooperatives, open-source system, or any policy intervention (Engle et al.).

Change management and organizational culture are quite essential in assessing success on adoption. Introduction of technology assumes the workflow redesign, the redefinition of roles, and, in certain instances, clumsy realization of the algorithms to be superior in certain tasks as compared to the human judgment. This is because those organizations that possess collaborative cultures, have a dedication to a leadership have the right training facilities and the forbearance towards initial adverse presentation challenges are more successful in adoptions. The models of implementation science that encourage the engagement of the stakeholders and the establishment of the continuous improvement and contextual flexibility may also increase the results of the implementation (Saboorizadeh et al., 2024).

Future Research Priorities

The direction of the research should also be provided in some directions. First, it is important to have a prospective validation research which involves the installed systems being put through the normal operating conditions. The available evidence is largely grounded on the controlled experiments; the data on the effectiveness in the conditions of real-world will contribute towards strengthening the evidence base and forming feasible expectations to a significant extent. The causal evidence is yet to be established and it may be described by pragmatic experiments when the sites with and without AI-automation are contrasted (Qin et al., 2023).

Second, mechanistic interpretability research is going to be given more consideration. The available black box models are only able to provide predictions as opposed to descriptions and this limits scientific knowledge and trouble shooting. Instead, building architectures which can be read by nature, or post-hoc modes of explanation in which their predictor is still valid and provides chemical explanations would be of value to the scientific community. There is some potential in the hybrid approaches to the combination of mechanistic knowledge and data learn method (Tang, 2025a).

Third, there should be a focus on the strength and quantifying uncertainties. Sound uncertainty estimates can be used to make proper human verification- high-confidence predictions automatically and low-confidence cases are then forwarded to human inspection. Estimation of uncertainty is also quantified with Bayesian techniques, ensemble techniques and conformal prediction, all of which are computationally expensive and seldom applied. With effective measures of uncertainty, the human-AI collaboration would be enhanced much better (Yousefi, 2025).

Fourth, the transfer learning and few-shot learning should be investigated. The high costs and big data are currently involved in the need to train AI models to be trained on cases that are difficult to compute (have a rare target) because they are targets of orphan diseases (radioisotopes with limited production) or are a rare target (radioisotopes with limited production). Methods capable of successful learning on small datasets through transfer between related problems or taking into account already existing chemical intuition can take extremely large jumps to the problems of current intractability (Korde et al., 2024).

Fifth, more realistic in the description of real decisions are to be constructed there. The current systems are generally concerned with the optimisation of each, (yield, potency) and practitioner at a number of conflicting objectives (efficiency, safety, cost, sustainability, regulatory compliance). Certain approaches to searching the means of drawing preferences explicitly would be more apt to discovering a compromise between AI suggestions and human values and realistic restrictions (Oyeniran, 2024).

Finally, an ethical and social implication, which must be studied in a systematic manner, is present. Either AI-robots may enlarge the existing imbalances, concentration of the powers of those institutions that are also well-endowed, or create employment in laboratories. Equity, access, and the effects on the workforce, and the potential problems of dual-use should be actively considered, rather than the implementation of technical development, which is implemented at the end of the day (Tiwari et al., 2024).

CONCLUSION

The current systematic review provides certain good bites of evidence to indicate that a paradigm shift in the sphere of radiochemistry and drug discovery entails incorporation of artificial intelligence and automated systems. Among the 106 peer-reviewed studies, having

a wide approach and application, there are recurring trends of highly efficient use (30-60%), highly accurate use (15-30%), faster (40-100-fold) and less costly (40-55%). Such benefits can be enhanced way beyond the optimality which implies that the existing practice is informed by the underlying redistribution of experimental practices. Notably, AI-autonomous systems comprise the suggestion that there is more synergistic influence than the aggregate influence of every of the separate performances. The foundation of this synergy is closed loop processes where AI-based decision making generates automated processes, and experimental findings keep on improving AI models. These self-enhancing systems will also introduce domain knowledge every one iteration, and will improve as it goes on.

The end of research demonstrations into practice should be directed at comprehensive spheres and the less complex obstacles should be discussed such as the creation of the regulatory framework, the data infrastructure, working staff training, and the economy sustainability. Even though the barriers might remain quite huge, the magnitude of the already demonstrated benefits and the accelerated development of technologies demonstrate that they are not only used by the multitude but also are rather an organic process. The first to it, institutions and organizations will gain benefits over their rivals, and perhaps establish growing divides between resource-based and resource-based environments on the ability to perform.

Rather than turning into some tested implementationer, the human factor under consideration turns into a more strategic decision-maker and a quality controller. This transformation entails the new skills that depend on domain expertise as well as the computational literacy and systems thinking-skills that the existing education programs do not provide appropriately. Reforming of curriculum and professional development programs as the tools of shaping this integrated skillset is the key to the facilitation of the technology adoption.

The tendency will be observed in the future: radiochemistry and drug discovery will be the property of AI and automation and not a solution of a professional. The issue now is not whether to introduce these technologies or not to do it, but how to do it, in a more or less fair and sustainable way. It ought to be proactive with regard to the transition of organizations, education, regulatory bodies and fund providers, through strategic investment in infrastructure, workforce, policies, closed research programmes, and collaboration to become ready.

Radiochemistry and drug discovery AI and automation is not a gradual expansion of the discipline, but is instead an entire redefinition of how we approach the breaking of the discovery platform and drug development. As these technologies continue to advance beyond the existing demonstration systems up to the next phase of full maturity of all their capabilities being the development of highly efficacious tested systems, they should serve to hasten the pace of innovations in the therapy, make radiopharmaceuticals more accessible, reduce the cost of development of the pharmaceutical business, and ultimately result in improved patient outcomes. This promise will require the realisation of other innovations in technology, rigor, reasonable application, and prioritising concern of equity and ethics to be put in the centre stage. Such transformative technologies may continue to play their part by revolutionizing the science of pharmaceutical and nuclear medicine to the good of all patients around the world or not, the next decade will tell.

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