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CD Chem Group
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Where synthesis meets intelligence

AI has accelerated and validated early-stage drug discovery; continuous flow chemistry now proves critical to accelerating the scale-up of those molecules, says **Subir Chakraborty** of **CD Chem Group**

In June 2025, Insiico Medicine reported Rentosertib, a small-molecule TNIK kinase inhibitor for idiopathic pulmonary fibrosis, that was identified end-to-end by machine learning (ML). A 71-patient Phase IIa trial published in *Nature Medicine* showed that the 60 mg daily dose improved lung function by approximately 98 mL compared to the placebo decline. The candidate reached clinical trial in roughly two and a half years. That milestone stands as proof of concept.

As of 2026, however, no drug designed by artificial intelligence (AI) has gained regulatory approval, and around 90% of candidates entering clinical development still fail, much the same as before.² AI has thus transformed early discovery economics without yet changing late-stage odds, where human biology, not chemistry, determines the outcome.

Bottleneck now upstream

A working AI pipeline for anti-cancer new chemical entities (NCEs) now runs in five stages (Figure 1):

1. Target identification via 'omics' (genomics, transcriptomics, proteomics and metabolomics) analysis
2. Generation of virtual libraries in millions of SMILES strings

3. ML-driven filtering on binding affinity and absorption, distribution, metabolism, excretion and toxicity (ADMET)

4. Synthesis and preclinical validation with results logged in electronic laboratory notebooks

5. Retraining of models on real bench data

Graph neural networks, diffusion models and reinforcement learning drive molecular design. AlphaFold 3 has transformed structure prediction.³ Teams report reaching a preclinical candidate in less than 15 months rather than the historical time of over five years before advancing to Phases II and III.

Critically, AI filtering applies probability scoring to each candidate: predictions that a compound has, for example, an 80% likelihood of viable oncology activity narrow millions of theoretical structures to 10–15 lead compounds for synthesis. This filtering step compresses the cost equation. Reducing screening burden mitigates the largest cost lever available in pharmaceutical synthesis: step count, cumulative yield loss and precious metal catalyst usage.

Synthesis still the challenge

Oncology NCEs are structurally demanding. Their cores are

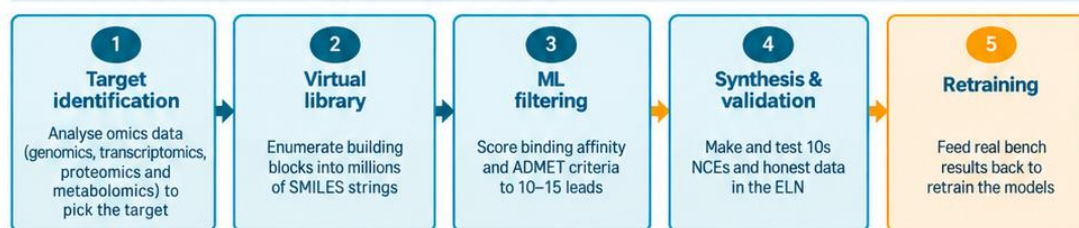
heterocyclic (quinazolines, pyrimidines, indoles), fluorination is widespread for metabolic stability and typical syntheses run to 10–20 steps. Many of these reactions are precisely those that batch processing handles least well.

Continuous flow chemistry addresses this directly (Table 1). Nitration is strongly exothermic and hazardous at scale in batch but flow reactor control removes that risk. Hydrogenation benefits from continuous hydrogen dosing and improved catalyst efficiency. Halogenation and fluorination gain precise reagent control and fewer side reactions. Cyclisation improves selectivity. Multi-step telescoping combines steps without isolating intermediates, compressing a 10–12-step synthesis into six to eight.

Since many oncology actives are high-potency APIs (HPAPIs) requiring containment, avoiding intermediate isolation also reduces operator exposure to cytotoxic material. Scale-up becomes time-based rather than volume-based, improving reproducibility for regulatory filing, whilst lower solvent use and reduced waste serve environmental, social and governance (ESG) objectives.

Liposomal encapsulation and next-generation delivery systems

Figure 1 - Closed-loop AI discovery pipeline for anticancer NCEs



Reaction type	The problem in batch	What continuous flow delivers
Nitration	Strongly exothermic; a safety risk on scale-up	Controlled heat removal and safer scale-up
Hydrogenation	Liquefaction in H ₂ flow inhibitors, catalyst handling and oven dosing are awkward	Continuous hydrogen dosing and better catalyst efficiency
Halogenation and fluorination	Common in modern oncology drugs; prone to side reactions	Precise reagent control and fewer side reactions
Cyclisation and heterocyclic formation	Challenging steps for quinazoline, pyrimidine and indole scaffolds	Improved selectivity and shorter reaction times
Multistep telescoping	Isolation of each intermediate adds cost and exposure to cytotoxic material	Steps combined without isolation; a 10 to 12 step route compressed to 6 to 8

Table 1: Key reaction types in oncology API synthesis & what continuous flow resolves

Like LipoHedge further extend the clinical value of AI-identified molecules, Liposomes protect drugs from degradation, improve cellular uptake, and reduce off-target toxicity. LipoHedge formulations incorporate targeted delivery mechanisms and enhanced stability.

Together, these technologies achieve lower, more tolerable doses, reduced systemic toxicity, extended circulating half-life, and passive tumour targeting via the EPR enhanced permeability and retention effect. This synergy between AI-designed molecules, continuous flow-synthesised actives, and advanced formulations is where competitive advantage now resides.

Market drivers

The commercial case follows the chemistry. Costs at given by step count, cumulative yield loss, precious metal catalysts, containment, infrastructure and regulatory compliance. Removing steps lowers the over-larger cost lever. The KPAPI market is forecast to grow from approximately \$25 billion in 2024 to nearly \$40 billion by 2029. Small molecules continue to account for the majority of novel drug approvals. This is not niche demand.

In January 2025, the US FDA issued its first draft guidance on AI in drug development, proposing a risk-based credibility framework. "Notably, it

excludes discovery itself, where a wrong prediction, merely results in waste of the experiment process. The regulatory focus falls on non-clinical, clinical, post-marketing and manufacturing applications.

Case study: AI compound analysis

Consider a compound identified through AI screening: SMILES notation C1NCCCNC(=O)C1CCCC1NC. Molecular weight calculates gives 279.3 g/mol, with a logP of 0.23. Balanced solubility. The topological polar surface area (TPSA) was 101.27 Å², supporting water solubility and oral bioavailability. All of these parameters satisfy Lipinski's rule of five, indicating drug-like properties.

ML models predict random-forest classifiers to score 82.5% anti-cancer probability, gradient-boosting models reach 93.1% and neural networks score 92.7%. The ensemble verdict is "likely anti-cancer," with 75% agreement across models. The next steps are definitive *in vitro* cytotoxicity assays on cancer cell lines, *in vivo* pharmacokinetic studies in animal models and computational modelling to optimise structure.

Outlook

Value from these developments will accrue not to general CDMOs, but to organisations that invest in data

infrastructure before models, keep experienced synthetic chemists in the loop, and connect powerful digital tools to supply chains that can actually deliver the compound. Continuous flow chemistry, advanced formulation, and AI-integrated discovery can help to solve the synthesis challenge.

The bottom line is that the molecule still has to be made and then is precisely where chemistry expertise, process innovation and manufacturing capability are required to compete in drug discovery.

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Subir Chakraborty
CEO

CD CHEM GROUP
subir@cdchemgroup.com
www.cdchemgroup.com



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