INSIGHTS

LESSONS FROM THE AIDDD CHEMISTRY TRACK

FROM PREDICTION TO PROOF

Constraints in molecular discovery have shifted decisively toward data generation, experimental throughput, and the ability to integrate computational models into real-world chemistry workflows as revealed in the Chemistry track at AIDDD 2025.

Rather than centering on novel algorithms or model architectures, there was a sense of pragmatism. Industry leaders returned to questions of execution: how AI is being operationalized inside organizations, where it meaningfully accelerates decision-making, and where friction persists. AI was framed not as a replacement for chemists, but as a collaborator whose value depends on how tightly it is woven into everyday scientific practice.

This report captures important insights from Chemistry Track at the AIDDD Summit 2025, with a focus on Hit Identification, Data Generation and best practices from leading teams.

FREDDIE METHERELL

PORTFOLIO DIRECTOR

FROM HIT IDENTIFICATION TO PRACTICAL PROGRESS

Sessions at AIDDD 2025 explored AI's expanding role in hit identification, molecular design, and structure-enabled discovery. These discussions reflected a field that has largely moved beyond proof-of-concept demonstrations. However, as the track unfolded, attention increasingly shifted downstream—toward what happens after hits are proposed.

Experts repeatedly noted that theoretical gains achieved in silico are often eroded during resynthesis, confirmation, and prioritisation. The challenge is no longer generating candidate molecules, but progressing them efficiently through experimental bottlenecks that sit outside the model.

One computational chemistry lead summarized the frustration: "Most of the value is lost after the hit list."

Miles Congreve, Chief Scientific Officer, Isomorphic Labs

WHERE AI VALUE IS BEING LOST

Throughout AIDDD, participants described a pattern: strong computational suggestions followed by delays in synthesis, limited assay bandwidth, or slow confirmation cycles. These gaps were framed as organisational and workflow issues, rather than failures of modelling.

Execution gaps, not algorithms, are eroding AI impact.

DNA-ENCODED LIBRARIES AND HIGH-THROUGHPUT SCREENING

As one senior pharma executive put it, DEL has become “a reliable way to get started, not a guarantee of where you end up.”

The absence of marketed DEL-derived drugs was framed as a lagging indicator rather than a verdict on the approach itself.

Discussions around DNA-encoded libraries reflected a notably mature and experience-driven perspective. DEL was rarely positioned as a disruptive breakthrough. Instead, speakers described it as a dependable entry point within a broader hit discovery toolkit—valuable, but not universally applicable.

The absence of marketed DEL-derived drugs was openly acknowledged, but several participants pushed back on its relevance as a performance metric. Product launches were repeatedly described as lagging indicators that obscure earlier value created in hit finding and lead generation.

Conversations turned to data quality. False positives were viewed as manageable through established filters and confirmation strategies. False negatives, however, were seen as a more structural limitation. DNA attachment effects and downstream confirmation challenges mean that apparent inactivity does not necessarily reflect true lack of binding—a nuance that complicates both human interpretation and machine learning training.

Several returned to this point. As one described it, false negatives are “the silent failure mode”, often reflecting assay artefacts or DNA attachment effects rather than true inactivity.

Experts cautioned against treating raw negative DEL data as ground truth. For certain targets, compounds may fail to confirm not because they lack activity, but because the DNA-conjugated format distorts binding or assay readouts.

Negative data requires context, not blind exclusion.

Views on iterative DEL approaches were mixed. Some participants described them as essential tools for hard targets or constrained intellectual property landscapes. Others highlighted diminishing returns once chemical diversity has been largely exhausted. The prevailing sentiment was that methodology alone does not determine impact—context, target biology, and downstream strategy matter more.

DATA GENERATION AS THE NEW BOTTLENECK

AI models are increasingly constrained by the availability, fidelity, and relevance of experimental data. Improvements in model architecture were widely viewed as incremental compared with the gains unlocked by better data generation.

High-throughput platforms capable of producing kinetic—not just endpoint—data were repeatedly highlighted as critical enablers. Measurements of on-rates, off-rates, and residence times were framed as more informative for real decision-making than single-point affinity metrics.

One biotech founder noted that access to real-time kinetic data “changes the internal conversation,” allowing teams to build confidence earlier rather than discovering liabilities downstream.

KINECTICS OVER ENDPOINTS

Real-time kinetic data was repeatedly cited as changing how teams prioritise compounds, particularly when translating predictions into experimental follow-up. What you measure defines what AI can learn.

Execution gaps, not algorithms, are eroding AI impact.

As model architectures commoditize, competitive advantage is shifting toward organizations that can generate large, proprietary, high-quality datasets and close the loop between prediction and experiment rapidly.

DOMAIN-INFORMED AI: BEYOND GENERIC MODELS

As one data science leader put it, the goal is no longer theoretical accuracy alone, but building systems “chemists trust enough to use every day.”

Several participants underscored the limitations of applying generic machine learning approaches to complex chemical and biological systems.

Leaders emphasized that models gain credibility and usefulness when they reflect underlying chemistry or biology, rather than treating molecules as abstract data objects.

LEADING TEAMS: WHAT THEY ARE DOING DIFFERENTLY

Across discussions, a consistent picture emerged of how more advanced teams are operating. AI is treated as infrastructure rather than experimentation, embedded directly into standard discovery workflows rather than run as isolated pilots.

Reducing latency between design and experimental confirmation was prioritised over marginal improvements in model accuracy. Teams described pragmatic combinations of physics-based methods and machine learning, selecting tools based on data availability and project stage rather than ideological preference.

KEY LEARNING

Leading organizations invest heavily in scalable, high-fidelity experimental platforms and view data generation as a strategic asset rather than a support function.

Execution discipline is the real differentiator.

WHAT TO LOOK FOR IN 2026

A near-term future defined less by algorithmic breakthroughs and more by execution discipline. AI is becoming a standard component of discovery, but its impact will depend on how effectively downstream bottlenecks are addressed.

By 2026, competitive differentiation is likely to hinge on the ability to generate and curate proprietary datasets at scale, tighter integration between computational and experimental teams, and workflows that allow humans and machines to iterate together in near real time

LOOKING AHEAD

The prevailing sentiment was not hype-driven optimism, but confident pragmatism: the tools are here, and advantage now lies in how effectively they are used.

AI impact will be earned operationally.

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