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Case Study

First Application of AI-Driven Small Molecule Synthesis in a Non-Pharmaceutical Industry

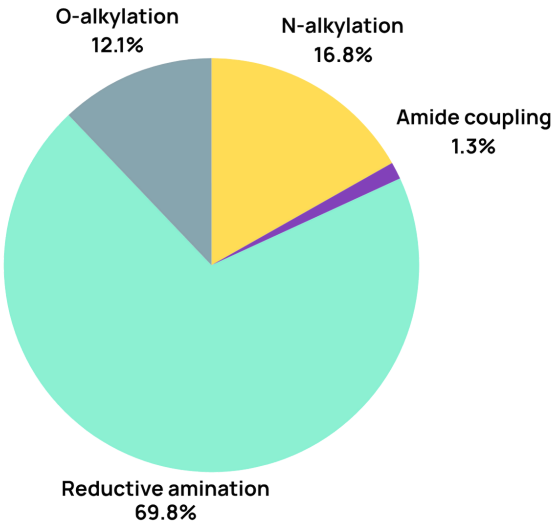
Challenge

Design and synthesis of unique **volatile compounds** with potential fragrance properties, achieving at least **90% purity** within tight time and budget constraints.

Molecule.one's solution: diverse custom on-demand space of molecules

The initial phase focused on client consultations to understand key requirements for the chemical structures: aromaticity specifications, functional group inclusions and exclusions, volatility parameters, and molecular size constraints.

Following these guidelines, we developed a customized library of **340,000 compounds** with high synthetic feasibility, readily available building blocks, and cost efficiency. The client subsequently identified **149 targets** from this collection for synthesis. The designed chemical space was accessible through four main reaction classes: predominantly reductive amination, followed by N-alkylations, O-alkylations, and amide couplings.



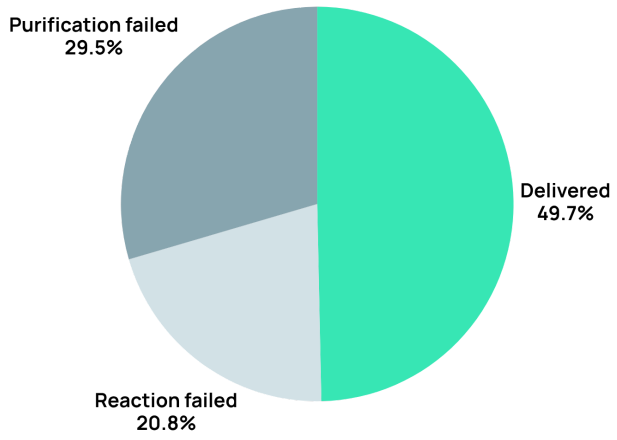
Data-Driven Extrapolation: Unlike conventional libraries constrained by fixed pharma building blocks, SpaceM1 is the first space constructed using deep-learning models trained on Molecule.one's proprietary HTE lab data. These models predict outcomes across diverse reagents and building blocks—without pre-selected sets—unlocking **unexplored regions of chemical space** with broad, accurate synthetic reach.

Success-fee based model: Molecule.one charged the customer only for compounds delivered successfully.

Results

Although reactions often yielded the desired products, purification—not synthesis—was the main bottleneck.
Most compounds were low-boiling, non-UV active, and difficult to handle using standard prep HPLC, leading to loss and re-purification cycles. To overcome this, we applied analytics-led triage: grouping compounds by key physicochemical properties and using LC-MS, GC-MS, and targeted staining to rapidly assess outcomes and prioritize purification effort where it paid off. This data-driven approach turned purification from a trial-and-error task into a structured, decision process, improving yield and reducing time. We leveraged here our culture and know-how to design a custom data-driven process that makes purification scalable not just for similar chemistries, but for millions of molecules.

Despite challenges associated with volatile and difficult-to-purify products, the overall synthetic success rate remained high at 79%, while 50% of all attempted reactions yielded screening-ready material meeting purity criteria.



To our knowledge, this represents the first application of small molecule design processes - typically used in early-stage drug discovery - to the fragrance industry.

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“Molecule.one delivered truly unique compounds.”

“Even within the well-explored regions of fragrance chemistry—built on familiar reactions and building blocks—they unexpectedly uncovered entirely new and interesting molecules.”

“The service matched, if not surpassed, the quality we receive from leading industrial suppliers, and the team demonstrated impressive precision in handling complex targets.”