

SOLVENT BLEND DISCOVERY ACCELERATED

DIGITAL R&D REDUCES LABORATORY WORK



EXECUTIVE SUMMARY

ACCELERATED INNOVATION

50+ SOLVENT BLENDS SATISFIED ALL END-CUSTOMER CONSTRAINTS IN 5 MONTHS

IMPROVED PERFORMANCE

150+ IMPROVED SOLVENT BLENDS DISCOVERED FROM OVER 100M CANDIDATES

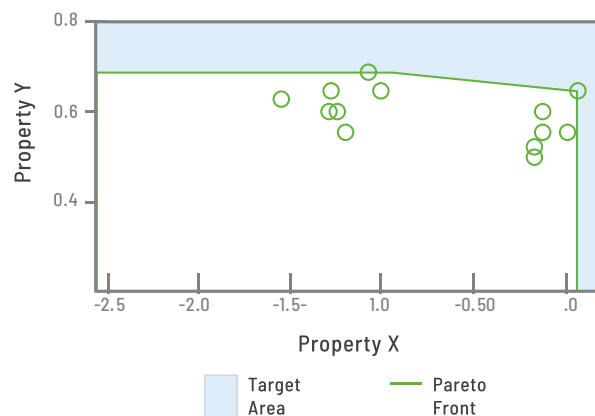
THE CHALLENGE

Solvent blends are needed by many different industries, with different end uses and target characteristics. Identifying suitable solvent blends through a process of synthesis and testing can be costly and time consuming.

The challenge for Citrine was to help Showa Denko target their testing efforts on candidate blends that had the highest chance of success—those that met all the downstream customer constraints and maximized the target properties. This was particularly challenging because none of the solvents in the initial training data set met **all** constraints and there were 850M+ possible combinations of the Showa Denko's in-inventory solvents.

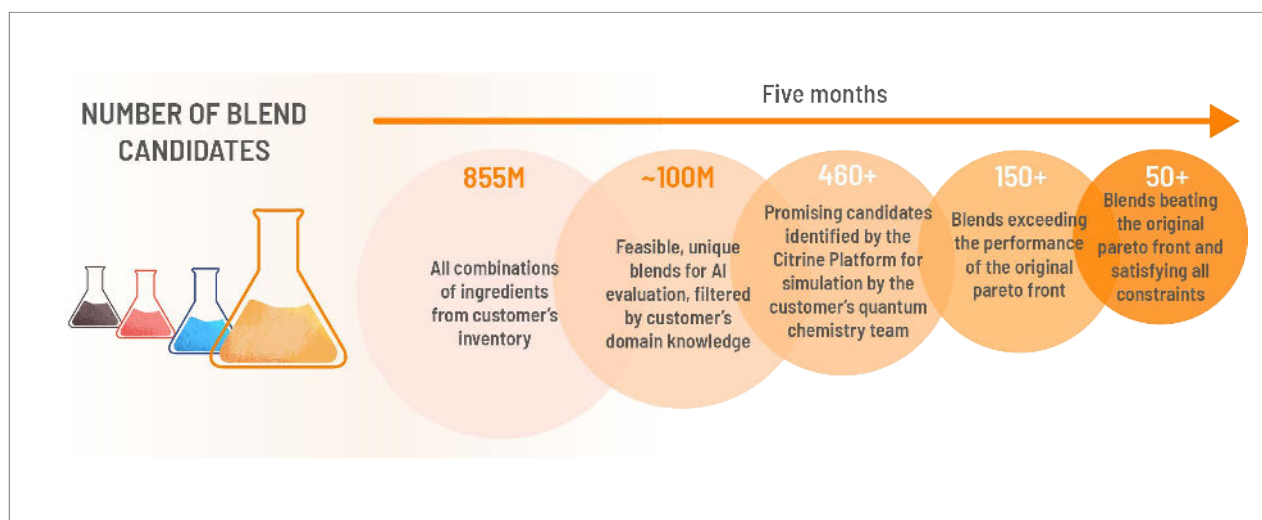
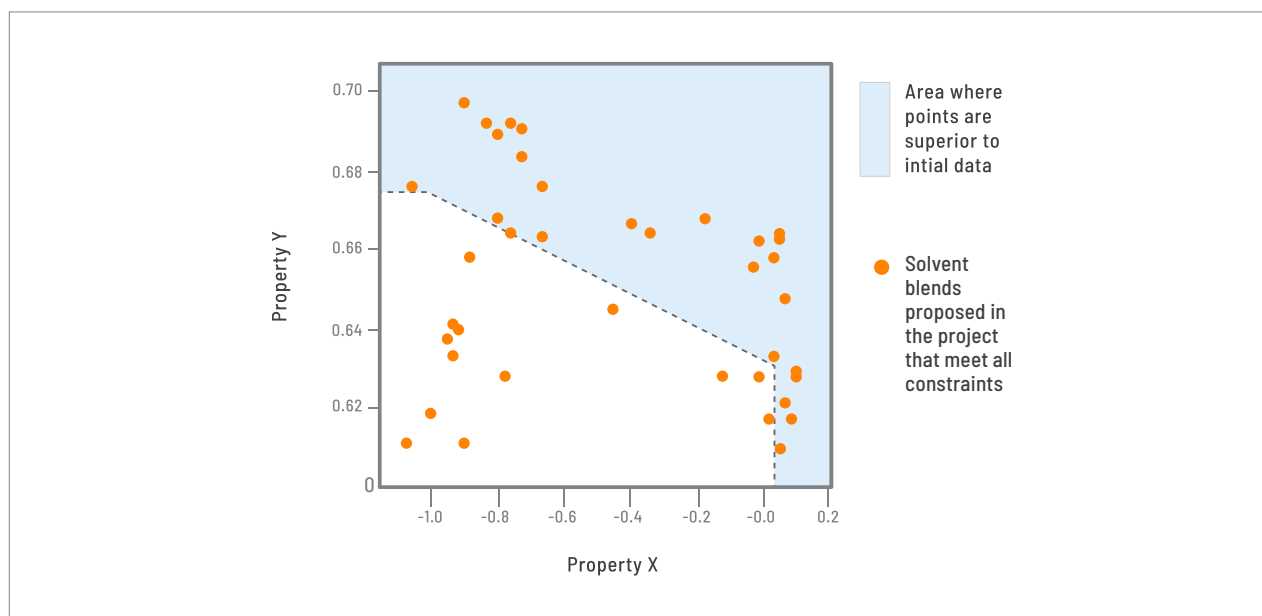
INITIAL DATA SET

None of the blends met **all** constraints



THE RESULTS

Just 5 months after starting the project, Citrine and Showa Denko had identified 150+ solvent blends that beat the original property pareto front (i.e. better than all previous results), based on quantum chemistry simulations. Over 50 of those blends satisfied all the project constraints. Showa Denko can now review the cost, risk, input materials, or constraints and property profiles of these potential blends and synthesize and perform confirmatory tests on their preferred candidates with their downstream customer.



FUTURE WORK

The Citrine Platform uses a modular graphical model so that components can be reused by future projects. Should the downstream customer requirements change, or a separate end-customer(s) request a similar project with a different requirements or trade-offs, the machine learning model could be quickly adapted to new target properties.

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