

Irish SME seeking to collaborate with experts in Pharmaceutical API small molecule crystallization, polymorph screening and solid-state analysis for Chemistry Manufacturing Control (CMC).

Summary

Profile type

Technology offer

Company's country

Ireland

POD reference

TOIE20250821014

Profile status

PUBLISHED

Type of partnership

Research and development cooperation agreement
Commercial agreement with technical assistance
Investment agreement

Targeted countries

• World

Contact Person

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Term of validity

21 Aug 2025
21 Aug 2026

Last update

21 Aug 2025

General Information

Short summary

A complication in pharmaceutical drug development process is polymorphism, the ability of a compound to exist in more than one stable crystalline structure & to switch form over time depending on different conditions. Different forms of drug molecule can have different properties making the medicine less effective, even unpleasant & harmful to patients. Crystal structure prediction tech is transformative for dealing with polymorphism to make drug development faster, more cost effective & less risky

Full description

Crystal Structure Prediction (CSP) offers a reliable digital in-silico method for solid state analysis of Active Pharmaceutical Ingredient (API) small molecules that can significantly enhance the understanding of a target molecule's physical properties and polymorphic landscape. CSP is best used in combination with experimentation for a right-first-time approach to drug form selection and de-risking which supports the achievement of regulatory approval and faster time-to-market for new medicines.

The company's predictive technology platform – CHEMINA – brings the power of digital simulation to the task of Crystal Structure Prediction (CSP) for new Active Pharmaceutical Ingredient (API) drug molecules.

The company goal is to provide deeper data insights for Drug Form Selection and De-Risking earlier in the drug development process and enhance work on API crystallization and solid-state analysis that is still heavily reliant on lab experimentation work.

As a result, the company enables smarter decision-making for pharma/biotech companies to get more candidate drugs to market faster with reduced risk. It is paramount that the results from the company's in-silico solution are transferable to concrete recommendations with respect to experimental work or valuable insights for our clients. The company's goal is to harness computational power and exploit in-silico methods to tackle challenges faced by experimentalists in the pharmaceutical industry.

The predictive technology platform is now commercially ready for deployment with pharma/biotech companies and CROs/CDMOs.

The company works with Pharmaceutical API small molecule development from early-stage lead optimization and pre-clinical studies through to Phase I-III studies for manufacturing and patent protection.

The company is seeking to collaborate with pharmaceutical / biotech companies and with contract labs (CROs/CDMOs) who are working on polymorph screening, crystallization studies and solid state analysis of API small molecules in order to deploy the company's predictive technology to enhance the overall drug development process.

Advantages and innovations

The company are driving innovation in the use of AI / Machine Learning, Quantum Physics and High Performance Computing (HPC) technologies applied to the highly specialized field of Crystal Structure Prediction (CSP) to dramatically reduce the risks and time-to-market for new drug development.

The company innovative molecular simulation platform CHEMINA provides the pharma/biotech industry with a fully integrated modular CSP solution that requires only the most basic 2-dimensional chemical structure of an organic molecule in order to predict and rank the full polymorphic landscape of lowest energy crystal structures for a target small molecule or Active Pharmaceutical Ingredient (API) compound.

This is achieved in particular through the use of AI (including Machine Learning and Neural Network technologies) together with Quantum Physics / Quantum Chemistry and High Performance Computing (HPC) technologies, to model the energies and forces of organic molecules for their crystal structures in a smart and targeted manner to address specific bottlenecks in the CSP process that improves the speed and accuracy of the overall results when compared to using empirical forcefield models or Density Functional Theory (DFT) methods only.

Technical specification or expertise sought

The company are seeking to collaborate with experts in Pharmaceutical API small molecule crystallization, polymorph screening and solid state analysis for Chemistry Manufacturing Control (CMC).

Stage of development

Already on the market

IPR Status

Secret know-how

IPR Notes

Sustainable Development goals

- **Goal 3: Good Health and Well-being**
- **Goal 9: Industry, Innovation and Infrastructure**

Partner Sought

Expected role of the partner

The company are seeking to partner with Pharmaceutical companies and with Contract Development and Manufacturing Organisations (CDMOs) working in the field of polymorph screening, crystallization studies and solid

state analysis of Active Pharmaceutical Ingredient (API) small molecules.

The company's ambition is to work collaboratively with the pharma/biotech company or CDMO partner to combine the in-silico predictive technology solution with their laboratory experimental capabilities to achieve an overall combined superior solution for right-first-time drug development which increases the speed to market and reduces the risk.

Type of partnership

- **Research and development cooperation agreement**
- **Commercial agreement with technical assistance**
- **Investment agreement**

Type and size of the partner

- **Big company**
- **SME 11-49**
- **R&D Institution**
- **SME 50 - 249**
- **Other**
- **SME <=10**

Dissemination

Technology keywords

- **06001015 - Pharmaceutical Products / Drugs**
- **03004007 - Pharmaceuticals**

Market keywords

- **05007002 - Pharmaceuticals/fine chemicals**

Targeted countries

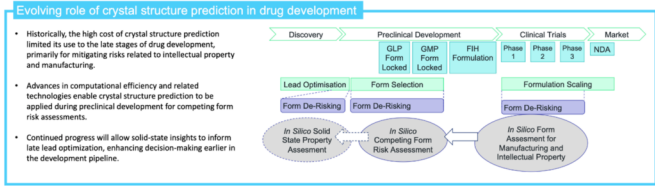
- **World**

Sector groups involved

- **Health**
- **Electronics**

Media

Images



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