

UCD's 2019 Start-up of the Year is BioSimulytics

[BioSimulytics](#) has won a €32,000 prize fund after being declared overall winner of the 2019 UCD VentureLaunch Accelerator Programme.

The aim of the annual UCD VentureLaunch Accelerator Programme, which is held at NovaUCD, is to support the creation and launch of sustainable and profitable new start-ups emerging from the University.

BioSimulytics is developing a software platform to bring greater speed, certainty and product data quality to a critical part of the drug development process.

Drug molecules are manufactured in their crystal structure but these structures are complicated by polymorphism, the ability of a compound to exist in more than one stable crystalline structure.

A simple ice (H₂O) molecule for example has 18 stable structures; drug molecules, which are considerably more complex compounds, can have hundreds of stable structures. In addition, a polymorph may change to a more thermodynamically stable form hours, weeks and even years later depending on conditions.

Polymorphic forms of a drug have different properties and can also differ in drug outcomes such as efficacy and toxicity. Finding and re-producing the precise and stable crystal structure of a new drug is essential, and is required for regulatory compliance as well as patent protection. It is an incredibly complex puzzle for drug manufacturers to solve, as out of tens of thousands of compounds only one may become a new drug suitable for patient use.

Currently experimentation is the method used by drug manufacturers to identify the correct crystal structure of a new drug. This is painstaking manual work which may take months to complete, and, in the end, the drug scientists may still be left wondering if all polymorphic structures were indeed identified.

Joining the dots (and atoms)

BioSimulytics is developing a software solution which only requires the basic 2-D structure of a compound to accurately predict the detailed profiles of all its polymorphic forms, ranked by the most stable, with full certainty achieved within weeks, resulting in a 20-50pc time saving on the current experimentation method. To do this the BioSimulytics platform uses a powerful combination of molecular chemistry, quantum physics, artificial intelligence and high-performance computing.

The members of the BioSimulytics team, a start-up emerging from the UCD School of Chemical and Bioprocess Engineering are, Professor Niall English, Dr Christian Burnham, Dr Pralok Samanta and commercial lead, Peter Doyle.

“We are delighted to have won the 2019 UCD Start-up of the Year Award which is testament to the hard work, dedication and progress of the entire team over the last number of years,” Prof English said.

“We are initially seeking to raise €400,000 in investment to build our core team to rapidly grow our business with leading pharmaceutical, biotech and CDMO companies globally.

“BioSimulytics is the result of collaborative research at UCD which has been funded to date by an Enterprise Ireland Commercialisation Fund, and I would like to thank Enterprise Ireland for their funding and support. I would also like to acknowledge the great encouragement provided by NovaUCD, the VentureLaunch facilitators, and specifically all of the VentureLaunch participants through their invaluable feedback and support during the programme,” Prof English said.

Pictured (from left): Peter Doyle, commercial lead with BioSimulytics with Professor Niall English and Dr Christian Burnham, UCD School of Chemical and Bioprocess Engineering. Photograph: Nick Bradshaw

Written by [John Kennedy](mailto:john.kennedy3@boi.com) (john.kennedy3@boi.com)

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