Next-generation digital platform for faster, more accurate and more predictable drug development

BioSimulytics provides a unique software solution using neural network technology and high performance computing for the accurate prediction of crystal structures of new drug molecules which addresses a complex challenge in the global pharma / biotech industry, and is a key platform technology for AI-enhanced drug discovery and development. Founded at the end of 2019 as a spin-out company from University College Dublin (UCD) in Ireland following substantial national scientific research funding, BioSimulytics secured its first commercial contract with a major European pharma company in Q3 2020 and has signed evaluation agreements with several others for further industrial validation of its technology as a disruptive innovation for drug development. The global structural biology & molecular modelling market was valued at over USD3billion in 2020 with a CAGR of 18.2% to 2025.

Market Problem – Solution Fit

BioSimulytics is focused on digitizing one particular but crucial step in the drug development process, which is key to how new drug molecules are brought to market in the form of pills. This requires finding the most stable crystal structure of the molecule, also known as the polymorph, because molecules can have many possible stable structures which are viable, and they can change over time from one stable structure to a different one, with different chemical properties, even after the drug has been manufactured and shipped for use.

This is potentially disastrous for a pharma company, and indeed there have been several cases of drugs been withdrawn from the market, such as the case of Ritonavir by Abbott Laboratories which cost the company an estimated loss of US$250M, due to problems with polymorphism. **Precise identification of the polymorph is now essential in regulatory and patent filings for new drugs**. The current state-of-the-art of experimental techniques for finding the most stable polymorph is a slow and arduous manual process, taking 6 months or longer, with uncertain results.

Breakthrough Technology

BioSimulytics has developed a digital solution to the problem. Our software platform can take the most basic 2D structure of a molecule, and running it through our algorithms, we can predict the full polymorph landscape of that molecule and rank the most stable crystal structures, all within a matter of weeks thus saving customers not only valuable time but most critically, providing them with much greater accuracy and certainty in the development process for new drugs. The race to develop vaccines for Covid-19 has demonstrated the powerful role that new digital AI- and HPC-based technologies can play in dramatically transforming the pharma value chain, and **BioSimulytics aims to be an important European player in this rapidly expanding global market** over the coming decade. The company has recently completed a pre-seed investment round involving a combination of national agency investment with strategic angel investors to support the growth of its product development team and client base in the EU and US, with a view to raising a Series A round in the next 24 months following full industrial validation of its technology.

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Contact for Further Information

For interested parties wishing to learn more, refer to:

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