

Technology Summary: Quantum Molecular Modelling for Drug Discovery and Materials Design

Opportunity Statement

Quantum Molecular Modelling is an emerging technology that harnesses the laws of quantum mechanics to accurately predict the chemical and physical properties of molecules and materials. The technology can significantly shorten lead times and increase success rates in development projects, including drug discovery, materials design (including biomaterials), and chemical process optimization.

Although commercial applications have been limited due to the high computational cost, recent developments and growth of GPU-based hardware and software have reduced the cost of adoption to the industry. As a result, there is potential for the technology to be used in rapidly growing markets such as drug discovery and biomaterials, which are expected to reach US\$71 billion by 2025 and US\$240 billion by 2027, respectively.

Therefore, there is an opportunity for companies and organizations to adopt this emerging technology to enhance their innovation capability in materials and drug development.

Techbridge Partner's Solution

Techbridge's Partner for this technology has developed proprietary software that has been tested in real-life applications and proven to significantly reduce the costs for compound screening without adversely affecting yields.

The key advantages associated with this technology are as follows:

- Increasing the hit rate from 0.1% to 10% compared to the traditional experimental method.
- Reduction in cost by up to 20 times

The Partner's track record and use cases include the following:

- Development of a drug candidate licensed to a global pharmaceutical company for US\$250 million.
- Development of a drug that passed Phase III clinical trial with a commercial value of US\$510 million
- Development of novel paints that bind to Mica surface to meet specific performance.
- Multiple drugs are currently in Pre-clinical and Clinical Trials developed with companies listed in ASX.

Collaboration Model

The Partner is seeking for collaborations in the following area:

- Consulting projects in the following area:
 - Drug Discovery
 - Material design
 - Simulation of Biomaterials for industrial applications including bioplastics
- Joint Development
- Licensing
- Test bedding

For additional information, please contact:

Innovation@tbv.sg

