Wales
Data Nation
Accelerator

AI based drug screening and docking studies to validate a new SME-academic collaborative research and product development pipeline

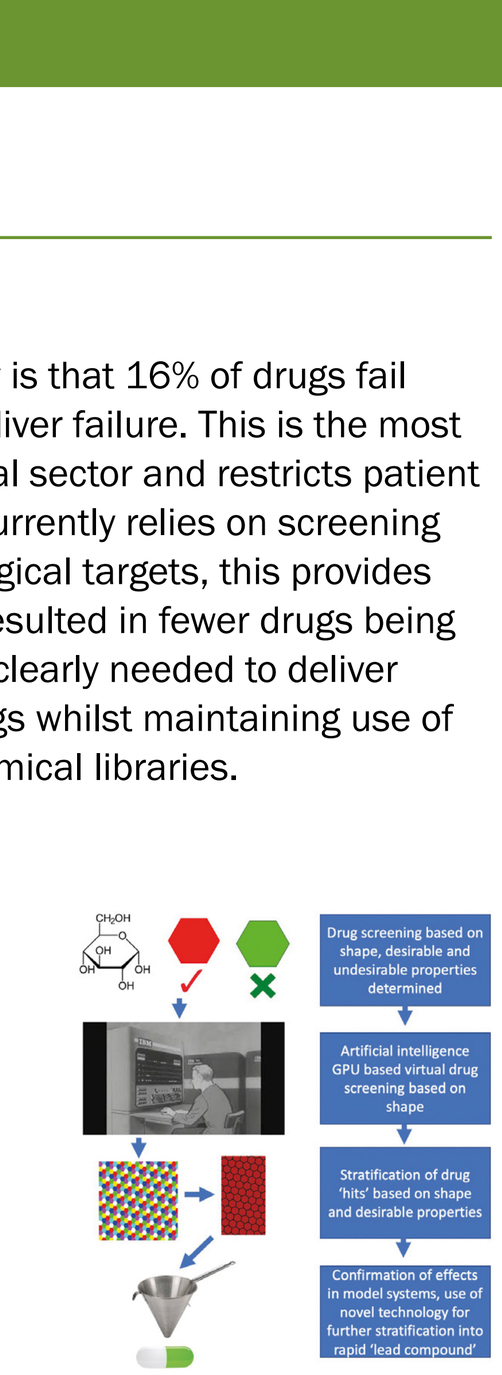
Summary

Challenge

A major challenge for drug discovery is that 16% of drugs fail safety studies because they induce liver failure. This is the most expensive cost to the pharmaceutical sector and restricts patient treatment options. Drug discovery currently relies on screening vast chemical libraries against biological targets, this provides no information on toxicity and has resulted in fewer drugs being developed. Improved strategies are clearly needed to deliver better, safer and more effective drugs whilst maintaining use of expensively developed in-house chemical libraries.

Solution

Artificial intelligence (AI) is being increasingly used to discover new drugs and tool compounds. One approach utilises high performance computing, namely graphics processing units, to screen compound libraries for chemicals similar in their 3D shape to the natural ligand or binding pocket of the target protein. We proposed a combined approach to utilise AI informed 3D shape based drug screening in two ways. First we screened sugar molecules for potential novel drugs impacting sugar metabolism, second we re-screened the hit drugs against the shape of drugs that cause liver toxicity. We ranked our compounds according to the least and most likely to be toxic and tested them in cells. Using magnetic purification technology developed by Liquids Research we were able to confirm that our AI approach worked and that we have generated a new and improved drug screening platform.



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Benefits/beneficiaries

1. Drug discovery scientists (academic and industrial) - Our novel pipeline, incorporating AI, once fully confirmed with additional experimental evidence, can be used to significantly improve the drug discovery process. This reduces time to identify lead compounds and screens out potentially toxic compounds, thus potentially reducing time to the clinic and considerably reducing drug discovery costs.
2. Liquids Research Ltd - Confirmation, via this project, of the utility of their novel superparamagnetic iron oxide nanoparticles for use in confirming the AI stratified on and off-target effects of drugs. This is a new and novel method that is potentially of great utility to the drug discovery industrial sector.

Difference made

A confirmation that it is possible to combine artificial intelligence led research with novel Wales-based biomaterials manufacturing science to produce a pipeline for improved drug discovery.

Further exploitation/next steps

Our aim is to now publish the pipeline, which will evidence our new AI based drug discovery method. This, in turn, is likely to enhance existing collaborations (e.g. with local and international companies), trigger new ones and lead to funding to further refine and use the approach. A natural progression is to develop the combined AI/biomaterials approach for testing the effects of drugs on other toxicology targets (e.g. the cytochrome p450 enzymes).

Project group

Company collaborators:

1. Liquids Research Ltd, Bangor, North Wales
2. SOM Biotech, Barcelona, Spain