Harnessing the power of AI to focus compound collections

A collaboration with Medicines Discovery Catapult

Medicines Discovery Catapult is a national facility connecting the UK community to accelerate innovative drug discovery. It brings together a fragmented sector of industry, academia, charities, technologists, services, finance companies, SMEs and start-ups.

BioAscent's collaboration with Medicines Discovery Catapult focused on the BioAscent Compound Cloud, which contains approximately 120,000 compounds. These can be accessed on-demand either as pre-selected focused libraries or custom libraries cherry-picked for a specific project; a vital resource for drug discovery for those looking for a rapid, customisable, IP-free and cost-effective solution. For example, those who do not have access to their own collections, or organisations looking for new chemical space beyond their in-house libraries.

Typically, compounds are tested against disease targets to identify the specific active compounds for optimisation. The active compound(s) then become the starting point for drug development.

Challenge:

Enabling biotechs and SMEs to purchase appropriate focused subsets from Compound Cloud – either preselected target class sets or sets completely tailored to the customer's requirements – will reduce initial purchase costs and downstream screening expenses. Ultimately helping to reduce the cost of drug discovery while also making it faster and more efficient.

Deciding which compounds to include in these subsets is, however, a challenge.

Solution:

Harnessing the power of AI and machine learning, Medicines Discovery Catapult's team have applied deep learning methods to analyse millions of compound bioactivities in order to learn which features of a compound make it active towards different drug targets and, ultimately, predicting the active compounds for potential drug development.
As part of a pilot project with BioAscent's Compound Cloud, compounds which were likely to be active towards different drug classes, such as kinases and GPCRs, were labelled. The approach was validated by successfully predicting the compounds within Compound Cloud already known to be active and affect a drug target.

Impact:

The application of this type of AI across the entire library has three significant benefits:

1. Adding value to BioAscent's compound library by highlighting likely bioactive compounds and as a rich source of high-quality bioactive molecules
2. Enabling creation of focused compound subsets or collections, grouped by for example likely therapy area
3. Supporting SMEs to conduct faster and more efficient drug discovery

Commenting on the collaboration, Phil Jones, CSO of BioAscent, said: "It has been great to access the Artificial Intelligence expertise at MDC for this collaboration. The MDC team have taken an innovative approach to characterising the compounds in Compound Cloud which we believe adds value to the collection and will benefit BioAscent's customers. From our perspective the collaboration was easy to establish and worked extremely well, and we look forward to working with MDC on further AI initiatives in the future."

To find out more please get in touch.

info@bioascent.com

+44 (0) 1698 534002