

Written by Matt Segall

Monday, 10 December 2018 14:23 - Last Updated Monday, 10 December 2018 14:39

---

Harnessing AI for drug discovery applications will significantly speed the identification of promising drug candidates, believes Matt Segall, CEO at Optibrium. The UK-based firm, together with partners Intellegens and Medicines Discovery Catapult, recently received a grant from Innovate UK to help fund a £1 million project focussed on combining Optibrium's existing StarDrop software for small molecule design, optimisation and data analysis, and Intellegens's deep learning platform Alchemite.

The aim is to develop a novel, deep learning AI-based method for predicting the ADMET (absorption, distribution, metabolism, excretion and toxicity) properties of new drugs candidates. Ultimately, the platform could help to guide the selection and design of more effective, safer compounds earlier in the discovery process...

## AI advances healthcare research



**SOPHIA KTOBI EXPLORES THE ROLE OF AI AND DEEP LEARNING IN HEALTHCARE IN THE FIRST OF A TWO PART SERIES**

Harnessing AI for drug discovery applications will significantly speed the identification of promising drug candidates, believes Matt Segall, CEO at Optibrium. The UK-based firm, together with partners Intellegens and Medicines Discovery Catapult, recently received a grant from Innovate UK to help fund a £1 million project focussed on combining Optibrium's existing StarDrop software for small molecule design, optimisation and data analysis, and Intellegens's deep learning platform Alchemite.

The aim is to develop a novel, deep learning AI-based method for predicting the ADMET (absorption, distribution, metabolism, excretion and toxicity) properties of new drugs candidates. Ultimately, the platform could help to guide the selection and design of more effective, safer compounds earlier in the discovery process, Segall states.

The pharma industry is increasingly harnessing sophisticated data science to

"The platform combines two-dimensional and three-dimensional structure activity relationships with de novo design, to help explore new strategies for optimisation"

A big pharma company might have one

You can link to the Scientific Computing World article [here](#)