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 focused on combining Optibrium’s existing StarDrop software for small molecule design, optimisation and data analysis, and Intellegen’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 drug candidates. Ultimately, the platform could help to guide the selection and design of more effective, safer compounds earlier in the discovery process...