How machines can design drugs

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Artificial intelligence (AI) is emerging as an important new approach to how new medicines will be designed. The first molecules designed by algorithm are heading for the clinic and we now have evidence on the impact AI technologies will have on the drug discovery process. Originally, spun out from his lab at the University of Dundee (*Nature* 492(7428):215-20), Exscientia is the first company to demonstrate the automation of drug design surpassing human endeavour. Whilst a wealth of machine-readable data in chemistry, pharmacology and biology is now available, drug discovery, especially for novel drug targets, where little or no pharmacology data exists, is by definition a "small data" problem. Moreover, the problem of data annotation (via experiments) is relatively slow and expensive. Slow and expensive. Here we will introduce how small amounts of seed data can be generated and how the development of active learning algorithms to learn efficiently from small data is the appropriate strategy to apply AI to the design of first in class drugs. The power of the approach will be demonstrated in cases studies of the pre-clinical drug candidates that have been designed by the system that are now in late stage IND-enabling studies. Exscientia's productivity metrics achieved on its first projects indicate the application of AI to drug discovery can potentially reducing the cost of bring a drug to market by 30%, approximately around $600m per licensed drug.