Table S1: Additional examples of AI used in preclinical stages of drug development

AI Technology utilised	Function of AI on which technology is based	Reference
Tessella	Predicts binding of molecules to form a stable compound	[1]
Exscientia	Predicts which molecules are capable of binding to their targets for specific disease states	[1]
HealNet	Assists with the discovery of and translation of new treatments towards clinical use	[1]
Derek for Windows (DfW)	Knowledge-based expert system capable of predicting chemical toxicity	[2]
Project Rephetio	Algorithm designed to identify patterns of efficacy and predict new uses for drugs	[3]
DeepChem and AutoQSAR	ANN-based systems that are designed to optimize the design of drug formulations	[4]
Markov chain Monte Carlo algorithm	ML applying Bayesian statistical approaches to characterise interindividual pharmacokinetic variability with pravastatin	[5]
SSnet	ANN-based system that relates protein structure to ligand information to predict protein-ligand interaction probability	[6]
KnowTox	*In silico* assessment of interactions, particularly induction of xenobiotic enzymes, endocrine effects, and liver toxicity	[7]
BioBERT and ClinicalBERT	Language modelling systems that are capable of mining through biomedical texts supporting information retrieval, text	[8]

	classification, text summarization and sentiment analysis	
ADRAlert	An ML driven technology that determines the strength of gene–ADR associations by statistically solving complex drug-gene–ADR network interactions	[9]

The AI technologies described in this table were obtained through the narrative review. They represent evidence of AI that has been successfully applied in industry or as proof of concept for the application of AI to a specific problem relating to drug development in the preclinical and R&D stages

Abbreviations: ANN – artificial neural networks; ML – Machine learning; ADR – adverse drug reaction

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