

Supplement

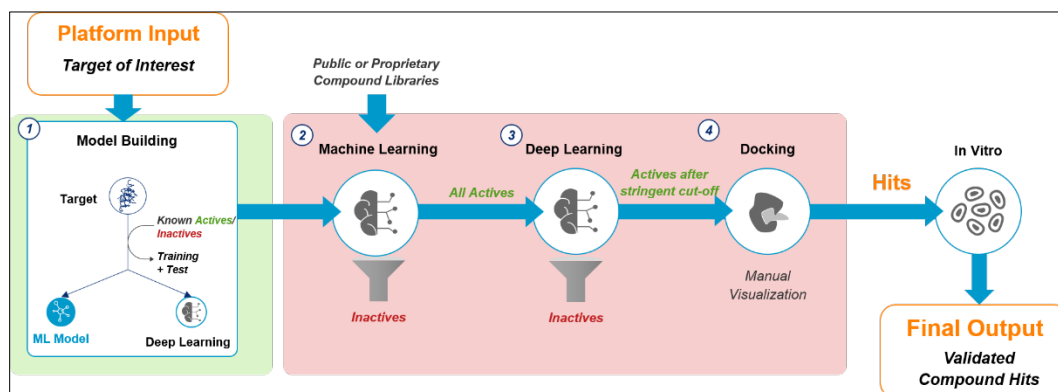


Figure S1. Excelra's Multi-layered AI Platform for Hit Identification

Total n= 52	Predicted: Yes	Predicted: No
Actual: Yes	12	3
Actual: No	8	29

Table S1. Confusion matrix for pipeline built for Bruton's Tyrosine Kinase

Additional reading on AI/DL/ML applications reported in pharmacometrics:

1. Yamashita F, Fujita A, Sasa Y, Higuchi Y, Tsuda M, Hashida M. An Evolutionary Search Algorithm for Covariate Models in Population Pharmacokinetic Analysis. *J Pharm Sci.* 2017 Sep;106(9):2407-2411.
2. Hall RG, Pasipanodya JG, Swancutt MA, Meek C, Leff R, Gumbo T. Supervised Machine-Learning Reveals That Old and Obese People Achieve Low Dapsone Concentrations. *CPT Pharmacometrics Syst Pharmacol.* 2017;6(8):552-559.
3. S Polak, A Mendyk, N Patel. Combining machine learning and mechanistic modeling approaches to solve real life problems – assessment of the local tissue binding and its influence on the systemic exposure after topical application of drugs. *J Pharmacokinet Pharmacodyn* (2018) 45:S3–S134.