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From HTS to Drug Candidate: AI-Powered Strategies for Early Drug Discovery

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Finding an ideal hit compound from high throughput screening (HTS) which will be optimized to a drug candidate is not a simple task. Currently, a very high and expensive failure rate in finding the reasonable lead series from HTS during the early-stage drug discovery is a bottleneck in drug development. Therefore, selecting meaningful compounds from a slew of commercially available compounds or designed through deep/machine learning is still a big challenge. Furthermore, the most critical aspect in the drug discovery is bridging the gap between *in vitro* and *in vivo*. We aim to narrow these gaps faced in drug discovery by balancing actual experimental SAR and SPR data which has been accumulated over the years. In addition, predicting and elucidating targets of compounds is not easy but crucial in order to understand the mechanistic behavior of a drug. We have applied NGS approach in order to overcome this hurdle. Through applying collective intelligence based on the accumulated information, we have successfully developed novel lead candidates. We are now moving on further utilizing AI based algorithms with images from phenomic screening to predict compounds' activities. Hence, combined *in silico* approaches have enhanced the overall quality of lead candidate development process.

Key words: Cheminformatics, bioinformatics, artificial intelligence, lead candidate, in silico