

Table S4: Examples of AI in drug manufacturing, drug repurposing, pharmacovigilance, and post-market safety monitoring

AI technology utilised	Function and subfield of AI on which technology is based	References
Vulcan	ML-based AI that facilitates the acquisition, exchange, and use of data in translational and clinical research using data exchange standards to promote interoperability across healthcare and drug development for evidence-based insights, patient engagement, and decentralised clinical trials.	¹
<i>Web Crawler Tool</i>	Python-based based web-crawler that analyses 46 web pages for pharmacovigilance purposes	²
<i>WEB-RADR</i>	Includes detailed information on medicinal products of 130 countries and links all pharmacists in public sectors to other participants of the healthcare system. It is capable of analysing the data for pharmacovigilance issues and act, if needed, allowing patients and healthcare providers to directly report adverse events on the WHO global ICSR database, Vigibase, via the Vigifow system	³
<i>ML algorithm for multi-label classification</i>	Supported by the LINCS L1000 database, this algorithm assesses approved drugs for novel therapeutic properties and repositioning potential based on transcriptome data	⁴

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 manufacturing, pharmacovigilance, repurposing, and safety monitoring.

Abbreviations: ML – machine learning; ICSR – Individual Case Study Report; LINCIS - library of integrated network-based cellular signatures

1. Macdonald JC, Isom DC, Evans DD, Page KJ. Digital Innovation in Medicinal Product Regulatory Submission, Review, and Approvals to Create a Dynamic Regulatory Ecosystem—Are We Ready for a Revolution? *Frontiers in Medicine* [Internet]. 2021 [cited 2022 Oct 6];8. Available from: <https://www.frontiersin.org/articles/10.3389/fmed.2021.660808>
2. Ang PS, Teo DCH, Dorajoo SR, Prem Kumar M, Chan YH, Choong CT, et al. Augmenting Product Defect Surveillance Through Web Crawling and Machine Learning in Singapore. *Drug Saf.* 2021;44:939–48.
3. Kalaiselvan V, Sharma A, Gupta SK. “Feasibility test and application of AI in healthcare”—with special emphasis in clinical, pharmacovigilance, and regulatory practices. *Health Technol.* 2021;11:1–15.
4. Xie L, He S, Wen Y, Bo X, Zhang Z. Discovery of novel therapeutic properties of drugs from transcriptional responses based on multi-label classification. *Sci Rep.* 2017;7:7136.