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Artificial intelligence implementation in pharmaceutical products lifecycle

Koshechkin K.A.[1], Lebedev G.S.[1], Fartushny E.N.[1], Orlov Y.L.[1, 2]*

[1] *The Digital Health Institute, I.M. Sechenov First Moscow State Medical University of the Russian Ministry of Health (Sechenov University), Moscow, Russia*

[2] *Novosibirsk State University, Novosibirsk, Russia*

* *y.orlov@sechenov.ru*

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Motivation and Aim: Artificial Intelligence (AI) meets more and more applications in biology, medicine, pharmacy challenging fundamental computational problems [3–5]. To examine systematically the overall approach for artificial intelligence implementation in pharmaceutical products lifecycle.

Methods and Algorithms: Published studies in PubMed and IEEEXplore were searched from inception to March, 2021. Studies were screened for relevant outcomes, publication types, and data sufficiency, and a total of 73 (1,2 %) out of 6131 studies were retrieved after study selection. Extraction of data was performed by authors according to PRISMA (http://www.prisma-statement.org), and the quality assessment was performed according to QUADUS-2 [1]. We reviewed pharmaceutical solutions (https://www.cyclicarx.com/, https://intervenn.com/, https://www.ibm.com/watson-health) and publications.

Results: The first two stages of literature search yielded 2617 hits from PubMed and 1466 hits from IEEEXplore. The volume of search results from Sechenov-AI Information System was 2048 publications in 446 journals. After screening titles and abstracts, we excluded 2837 studies for duplication and 2745 studies for non-relevant abstracts or publication types. A total of 549 studies went through full-text review, of which 189 studies were excluded for result that was not of interest and 215 were excluded for insufficient data for analysis. After further exclusion, only 154 studies were retrieved after the second stage of literature selection. The third stage of literature review, and 23 studies were added, which result in 73 studies retrieved after literature selection, resulting in a total number of included 177 AI implementations for final analysis. All of Artificial Intelligence systems could be divided in multiple overlapping categories. For the total of 177 projects found the most popular area of AI implementation is Clinical trial and preclinical tests (34 %). On the second place stood the Novel small molecules design systems with 33 % from total. The third most popular scope for AI implementation is Target identification for novel medicines. More than 25 % of the systems provide this functionality. It is interesting that most of the systems specialize in only one area (102 systems – 57 % are single purpose). None of the systems provide functionality for full coverage of the lifecycle and function in all categories of the tasks. We reviewed also COVID-19-related applications of AI (in predicting respiratory failure, prognosis of patients) [2]. COVID-19 pandemic has evaluated novel chemical and biologic entities as potential therapeutics for SARS-CoV-2 infection, the repositioning and off-label use of existing agents approved for unrelated conditions is

widely advocated as a therapeutic approach against COVID-19 as it offers more rapid, actionable interventions against the virus.

Conclusion: This meta-analysis demonstrated that Artificial Intelligence solutions in Pharmaceutical Products Lifecycle could find numerous implementations, and none of the market available solutions cover them all. Natural Language Processing could be used for real world evidence-based trials, reports and summaries generation. Artificial Intelligence methods could be used for large amount of unstructured information analysis for new drug targets identification as well as novel molecules *generation in silico* and their activities prediction. Drug repositioning and repurposing could be done with text mining. Clinical trials utilize real world evidence with Artificial Intelligence support. Image classification can automatically discover, generate, and learn features of images which is useful in preclinical and clinical trials results processing. Artificial Intelligence aided Personalized therapy is used for risk prediction, and multiple factors analysis including genetics. Drug dispense control helps to discover counter indications and drug combinations interactions.

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