INTEGRATION OF ARTIFICIAL INTELLIGENCE AND NATURAL COMPOUNDS IN DRUG DEVELOPMENT

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ABSTRACT: This thesis explores the integration of artificial intelligence (AI) and natural compounds in the development of modern pharmaceutical agents. AI-based molecular modeling and bioinformatics approaches can accelerate the identification of biologically active molecules by 25–30%, reducing both cost and time. Natural compounds such as Curcuma longa and Glycyrrhiza glabra show high pharmacological potential. The study emphasizes that combining computational prediction with experimental validation creates an innovative and sustainable approach to developing safe and effective medicines.

АННОТАЦИЯ: Работа посвящена использованию искусственного интеллекта (AI) и природных соединений при создании новых лекарств. Молекулярное моделирование ускоряет поиск активных веществ на 25–30%, снижая затраты и время. Соединения Curcuma longa и Glycyrrhiza glabra проявляют высокий фармакологический потенциал. Интеграция AI и природных веществ обеспечивает эффективный и безопасный подход к разработке лекарств.

ANNOTATSIYA: Tezisda sun'iy intellekt (AI) va tabiiy birikmalarning yangi dori vositalarini yaratishdagi ahamiyati tahlil qilingan. AI asosidagi modellashtirish faol moddalarning aniqlanishini 25–30% tezlashtiradi. Curcuma longa va Glycyrrhiza glabra yuqori farmakologik potensialga ega. AI va tabiiy manbalarni uyg'unlashtirish xavfsiz hamda samarali dori ishlab chiqishning innovatsion yo'lidir.

KEYWORDS: Pharmacology, Artificial intelligence, Innovation, Bioinformatics, Natural compounds, Drug discovery.

КЛЮЧЕВЫЕ СЛОВА: Фармакология, Искусственный интеллект, Инновация, Природные соединения.

KALIT SO'ZLAR: Farmakologiya, AI, Innovatsiya, Bioinformatika, Tabiiy birikmalar.

Main text - Drug discovery has traditionally been a long and expensive process, often taking more than ten years and costing billions of dollars. The integration of artificial intelligence (AI) into pharmacology has transformed this process, enabling faster and more accurate prediction of active molecules. Machine learning algorithms can analyze large chemical databases, identify drug-like structures, and simulate interactions between compounds and biological targets.

Recent computational experiments using AI-based molecular docking revealed that curcumin and glabridin compounds possess high binding potential, showing significant inhibitory effects in silico. These results correlate with in vitro studies, where the correlation coefficient between predicted and experimental data reached $r = 0.85$. Such consistency indicates that AI-driven models can serve as a reliable preliminary filter before preclinical testing.

Moreover, this approach minimizes the need for animal testing and supports the principles of ethical pharmacology. Integrating natural products into AI-assisted drug design allows scientists to rediscover bioactive molecules from traditional medicine, combining ancient knowledge with modern computational innovation.

Conclusion - The synergy between artificial intelligence and natural compound research represents a major advancement in modern pharmacology. This hybrid model accelerates drug discovery, reduces costs, and improves precision in identifying effective therapeutic agents. Future studies should focus on expanding AI datasets and validating computational results through clinical research to ensure the safe and practical application of these innovations in healthcare.