Potential For Drug Development Using Artificial Intelligence and Machine Learning

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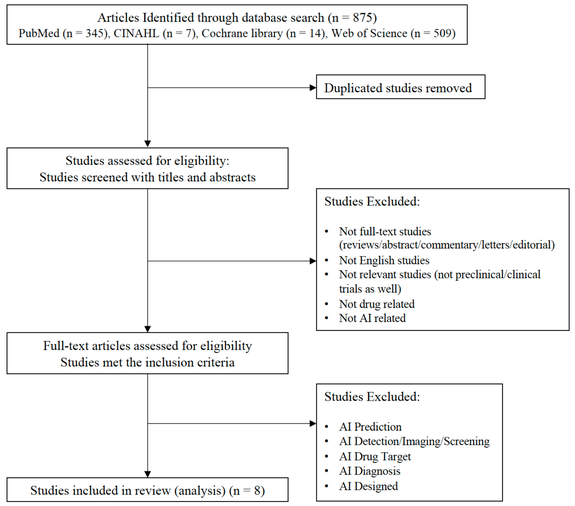
INTRODUCTION

Using AI and ML- learning in drug discovery has grown significantly over the last few years, aiding in target identification, drug design, repurposing, safety prediction, clinical trial optimization and data analysis. These technologies enhance efficiency, accuracy, and personalized medicine approaches, transforming drug development.

OBJECTIVE

This study aims to systematically review and evaluate the efficacy of AI- and ML-based substances as potential candidates for new drugs.

METHODS



To identify pertinent studies, articles published up to May 2023 were retrieved from databases such as PubMed, CINAHL, Cochrane Library, and Web of Science, utilizing relevant keywords. Following the PICO (Population, Intervention, Comparator, Outcome) framework and adhering to Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) recommendations, this study included articles evaluating the efficacy of AI- and ML-based substances in clinical trials.

RESULTS

Table 1. Summary of Study Characteristic

Authors	Intervention	Target Disease	Experimental Environment	Subject
Casey et al.	Peptide (pep_1E99R5)	Type 2 diabetes	in vivo	KK-Ay model of obese insulin-resistant DM
Kennedy et al.	Peptide (pep_RTE62G)	Anti-ageing	in human	Healthy female with visible periorbital wrinkles
Chauhan et al.	Peptide (NRT_N0G5IJ)	Type 2 diabetes	in vivo	6–7-week-old male db/db mice
			in human	Healthy males and females with Prediabetes
Wu et al.	Peptide (DP7)	Microbial infections	in vivo	6 to 8 weeks old male BALB/c mice
Kennedy et al.	Peptide (rice NPN)	Inflammatory	in human	65–75 years old Healthy males and females with BMI <30 kg/m2
Vidovic et al.	Molecule (TKA001)	Cancer	in vivo (C. elegans)	Not reported specific animal
Salim et al.	Molecule (COTI-2)	Cancer	in vivo	NCr-nu mice
Jiang et al.	Molecule (TMEA)	Thrombocytopenia	in vivo	Irradiation (IR) mice, C57BL/6N-TPORem1cyagen (Tpor-/-) mice

Table 2. Study Design and Outcome

Authors	Dosing	Compare Group	Result
Casey et al.	12.7 mg/kg (10 μM) or 63.5 mg/kg (50 μM)	Control groups of vehicle or Liraglutide (250 μg/kg)	Reduce HbA1c levels
Kennedy et al.	Emulsion 10, 25 or 35 ppm to each half of the face twice daily for 28 days	Emulsion alone	Changes in cutaneous relief parameters average roughness (Ra), average relief (Rz) and maximum relief amplitude (Rt) (anti-aging effect), Collagen density
Chauhan et al.	400mg/kg	Purified water (control), Rosiglitazone (15 mg/kg), Unhydrolyzed material (400 mg/kg)	Body weight and Fasting Blood Glucose
	15 g mixed and dissolved in 200 mL of water	Placebo (Avicel PH Microcrystalline Cellulose), Protein hydrolysate control (rice NPN) group	HbA1c concentration, postprandial glucose/insulin, BMI, weight, and fructosamine and fasting plasma glucose
Wu et al.	20 to 60 mg/kg IP Injection	20 to 60 mg/kg HH2 and 20 mg/kg Vancomycin	Reduce CFU count in the S. aureus
Kennedy et al.	10 g dose supplied in a pre-weighed sachet mixed with 200 mL water	Maltodextrin (Placebo)	Primary: Digestive discomfort Secondary: Decrease in serum circulating TNF-α, improved glucose control, decrease in serum LDL concentration, increase in HDL concentration
Vidovic et al.	100 μM and 200 μM	0.2% DMSO	Survival Probability (increased lifespan of C. elegans)
Salim et al.	IP: 3 mg/ kg, 8 mg/kg, 10 mg/kg IV: 20 mg/kg PO: 75 mg/kg	12.5 mg/kg of Paclitaxel, 3 mg/kg of Cisplatin	Tumor growth delay in 5 tumor xenograft models in mice (HT-29 colorectal cancer, SHP-77 SCLC, U87-MG glioblastoma, MDA-MB-231 breast cancer, and OVCAR-3 ovarian cancer)
Jiang et al.	2.5, 5, 10 mg/kg	Saline, TPO (3000 U/kg)	Promoted platelet regeneration

RESULTS

The search strategy yielded 663 articles after removing duplicates, and eight studies met our inclusion criteria. Encompassing a variety of diseases and conditions, these studies examined the efficacy of peptides and molecules discovered through AI and ML.

Table 1 provides an overview of the design of the studies. Most of the studies were conducted recently in 2023, 2021, 2020, 2016, or 2014. Each studies focused on specific subjects and disease as examining the efficacy and potential of the newly identified peptide or molecule using AI and ML- learning in vivo or in human.

As Table 2 illustrates detailed findings and among the eight articles, two studies investigated the effectiveness of discovered peptides in treating type 2 diabetes by assessing changes in HbA1c levels. Another study validated a peptide's potential for treating microbial infections by observing colony forming units (CFUs) in bacterial samples. Additionally, two studies identified promising molecules for cancer treatment, assessing survival probability and tumor growth. One study validated a drug molecule for thrombocytopenia by measuring platelet regeneration. Lastly, two peptides targeting anti-aging and inflammation markers. These evaluation included their effects on anti-aging and changes in TNF-α, glucose level, and serum LDL and HDL concentrations.

DISCUSSION

Notably, all peptides and molecules included in our analysis demonstrated efficacy in addressing their respective targeted diseases, and the subjects well-tolerated each peptides and molecules, which highlights their safety.

CONCLUSION

Although AI and ML in drug discovery are in early stages, the findings of this study suggest their potential to revolutionize the pharmaceutical industry and healthcare by accelerating drug development through the identification of unexplored molecules.