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Repurposing antihyperlipidemic drugs beyond lipid lowering: *In silico* approach into its GLP-1 receptor modulator potential

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ABSTRACT: Drug repositioning has recently become a crucial tool for discovering new biological effects of clinically used drugs. This study investigated the GLP-1 receptor modulator activity of antihyperlipidemic drugs, which are widely used by diabetic patients and those with cardiovascular diseases. The study was conducted using CB-Dock, an internet-based molecular docking program. The binding energies (kcal/mol) of the selected antihyperlipidemic drugs to the GLP-1 receptor were calculated, and Danuglipron was used as a reference compound. A comparison of the binding energies revealed that both the binding energy and localization of Ezetimibe were highly comparable those of Danuglipron. Following this analysis, the physicochemical and toxicological properties of Ezetimibe, the most potent compound, and Danuglipron were compared computationally. Docking analyses suggest that while Danuglipron engages the GLP-1 receptor through a canonical orthosteric binding mode, Ezetimibe preferentially occupies a more superficial cavity consistent with a potential allosteric modulatory interaction. This distinction highlights mechanistic differences between peptide-mimetic agonists and repurposed small-molecule candidates

KEYWORDS: Drug repurposing; ezetimibe; antihyperlipidemic; GLP-1 receptor; docking.

1. INTRODUCTION

The glucagon-like peptide-1 receptor (GLP-1R) has attracted considerable scientific interest in recent years owing to its involvement in body weight regulation. GLP-1R, a member of the G protein-coupled receptor (GPCR) family, is widely distributed across various cell types in the human body [1,2]. Its endogenous ligand, The glucagon-like peptide-1 (GLP-1), is a peptide hormone derived from the enzymatic cleavage of proglucagon. This hormone is primarily synthesized by L-cells in the intestinal mucosa, α-cells in the pancreatic islets, and neurons within the nucleus of the solitary tract. GLP-1 plays a pivotal role in maintaining glucose homeostasis and lipid metabolism [3,4]. Type 2 diabetes and its accompanying obesity are among the most significant threats to public health worldwide. Currently used medications are inadequate in some cases and do not have a significant effect on weight loss. This hinders the diabetes treatment process. GLP-1 agonists are showing promising results in overcoming this problem. These agonists enhance insulin secretion, suppress glucagon release, slow gastric emptying, and decrease food intake via central appetite regulation. Through these multifaceted mechanisms, GLP-1 signaling contributes significantly to obesity treatment. However, the clinical use of native GLP-1 is limited by its rapid degradation in the circulation, as it remains stable for only 1–2 minutes before being hydrolyzed by dipeptidyl peptidase IV (DPP-4) [5–7].

Clinically approved GLP-1 receptor agonists, such as Liraglutide and Semaglutide, are currently used for the management of diabetes and obesity through subcutaneous administration. Although these agents demonstrate strong therapeutic efficacy, their injectable nature poses limitations for patient convenience and compliance. In contrast, orally administered formulations offer distinct advantages, including greater ease of use and consistent dosing. However, recent advances in formulation technology and peptide engineering have enabled the development of orally available GLP-1 receptor agonists that maintain comparable bioactivity to

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their injectable counterparts. An oral formulation of the peptide-based GLP-1 receptor agonist Semaglutide has recently gained approval for the treatment of type 2 diabetes mellitus (T2DM) [8]. This peptide-based drug is co-formulated with sodium caprylate to enhance its oral bioavailability. It is administered once daily on an empty stomach, which necessitates a higher total dose compared with the once-weekly injectable formulation. The strong therapeutic efficacy of GLP-1R agonists in managing globally prevalent conditions such as diabetes and obesity has driven the pursuit of novel small-molecule candidates with similar biological activity. The remarkable therapeutic efficacy of GLP-1R agonists in managing globally prevalent diseases such as diabetes and obesity has intensified efforts to identify novel small-molecule alternatives.

In this context, Griffith *et al*. at Pfizer developed a non-peptidic GLP-1R agonist, Danuglipron (Figure 1), designed to replicate the beneficial effects of peptide-based drugs [8]. Although clinical studies demonstrated its efficacy in promoting weight loss and its potential utility in diabetes management, further development of Danuglipron was discontinued due to unexpected hepatotoxicity [9].

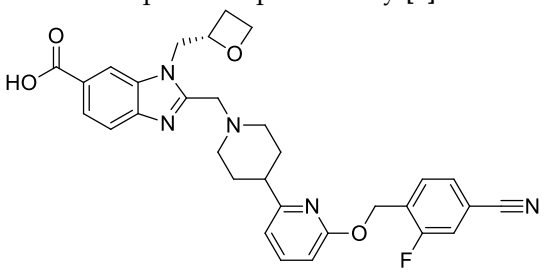


Figure 1. Structure of Danuglipron

Given these challenges, the development of novel, safe, and orally bioavailable GLP-1R agonists has become increasingly important. Nevertheless, the discovery of new drug entities is a lengthy and expensive process, often hindered by unpredictable toxicity and low clinical success rates. Although several candidate molecules, such as Danuglipron, have shown promising pharmacological efficacy, many fail to progress to approval due to adverse or unforeseen side effects. Small-molecule ligands targeting GLP-1R may engage the receptor through distinct binding mechanisms. While compounds such as Danuglipron are designed to mimic endogenous peptide agonists and interact with the orthosteric binding site, structurally diverse small molecules may exert their effects through alternative, non-orthosteric cavities. Such allosteric interactions have the potential to modulate receptor activity without directly competing with endogenous ligands, offering a mechanistically distinct approach to GLP-1R regulation.

In response to these limitations, drug repositioning has emerged as an attractive strategy in modern drug discovery. This approach seeks to uncover new therapeutic applications for existing drugs that already possess well-characterized safety and pharmacokinetic profiles. Repositioning not only reduces development time and cost but also mitigates the risk of unexpected toxicity. This strategy is particularly relevant for patients with metabolic or cardiovascular disorders, who often require multiple medications such as antihypertensive or antihyperlipidemic agents. Identifying additional therapeutic benefits within these drug classes may reduce polypharmacy, simplify treatment regimens, and improve patient adherence[10,11]. Antihyperlipidemic drugs represent a particularly relevant class for GLP-1R–oriented drug repositioning. Dyslipidemia, obesity, and type 2 diabetes are metabolically interlinked conditions that frequently coexist in the same patient population. Consequently, antihyperlipidemic agents such as statins, fibrates, and cholesterol absorption inhibitors are routinely prescribed to patients who are also candidates for GLP-1–based therapies. Several members of this drug class have been reported to exert pleiotropic metabolic effects beyond lipid lowering, including modulation of glucose homeostasis, insulin sensitivity, and inflammatory signalling. Moreover, their chronic oral use, established safety profiles, and favourable pharmacokinetic characteristics make antihyperlipidemic agents attractive candidates for repurposing toward additional metabolic targets such as GLP-1R.

In silico approaches offer valuable insights during the early stages of drug research. By calculating the binding energies between ligands and target receptors or enzymes, these methods provide significant contributions to the field of drug repositioning [12]. The aim of this study is to investigate the potential of clinically approved antihyperlipidemic drugs as modulators of GLP-1R using an in silico molecular docking and absorption, distribution, metabolism, excretion, and toxicity (ADMET) profiling approach. By comparing their binding affinities and interaction patterns with those of the small-molecule GLP-1R agonist Danuglipron,

this study seeks to identify repurposing candidates with favorable receptor engagement and drug-likeness properties for potential metabolic applications.

2. RESULTS & DISCUSSION

2.1 Calculation of Binding Energies

In this study, the binding energies (in kcal/mol) of nine clinically used antihyperlipidemic agents, proposed as potential GLP-1R modulator, were investigated through *in silico* molecular docking simulations. The evaluated compounds were Atorvastatin, Pravastatin, Rosuvastatin, Simvastatin, Fluvastatin, Ezetimibe, Fenofibrate, Gemfibrozil and Niacin (Figure 2).

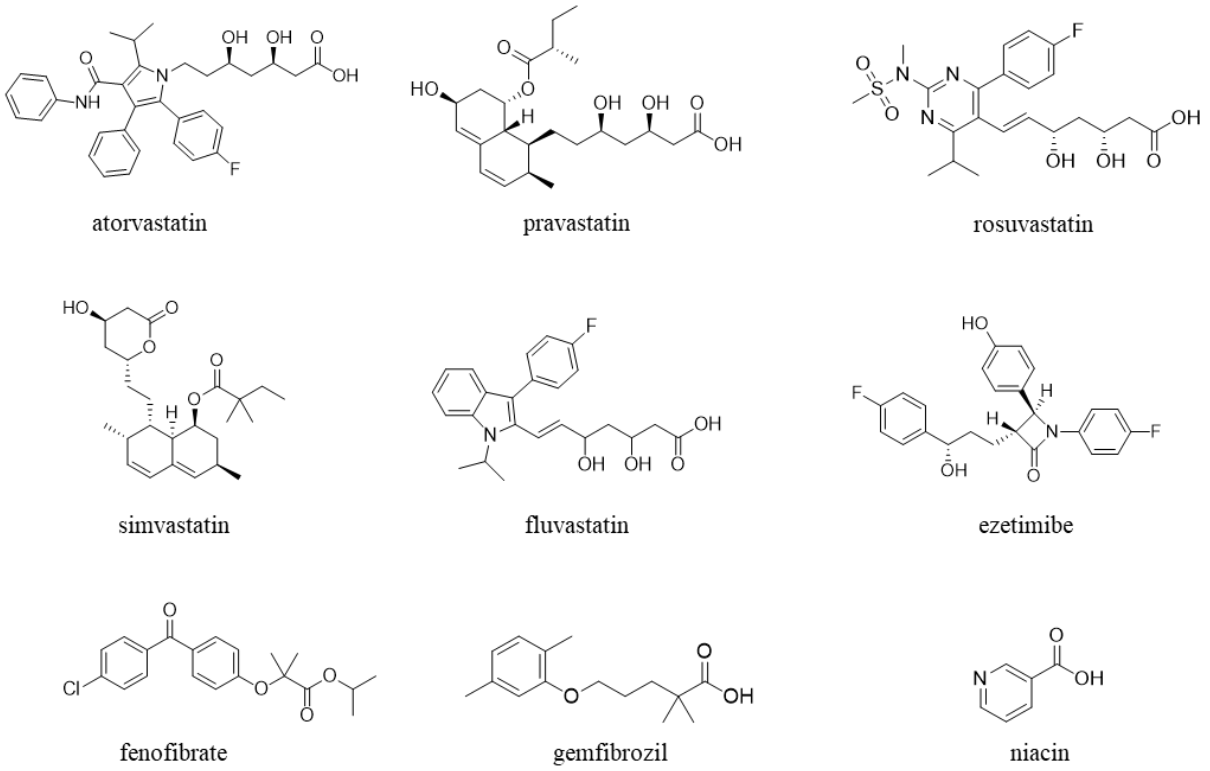


Figure 2. Molecule structures of nine antihyperlipidemic drugs

Binding energies approaching zero correspond to weaker interactions, whereas more negative values reflect stronger binding affinities. For investigation of specifically the modulator potential of nine antihyperlipidemic drugs on the GLP-1R, their binding energies were calculated (Table 1). According to the results of the blind docking analysis, the most favorable binding affinities were identified in the C1, C2, and C3 pockets of the Danuglipron molecule. C1, C2 and C3 pockets were identified by CB-docking program. Among these, the C1 pocket exhibited the strongest binding interaction, with a calculated binding energy of −13.8 kcal/mol. Based on these observations, the binding energies of the corresponding C1, C2, and C3 pockets in the investigated antihyperlipidemic drugs were subsequently computed. Since the C1 pocket of Danuglipron displayed the most stable binding configuration, comparative evaluations among the studied compounds were performed with respect to their C1 pocket interactions.

When the binding energies at the C1 pocket were compared among the studied drugs, Ezetimibe exhibited the closest binding affinity to Danuglipron, with a calculated energy of −9.0 kcal/mol. The binding energies of ezetimibe in the C2 and C3 pockets were also evaluated and determined to be −8.9 and −11.1 kcal/mol, respectively. These values were highly comparable to those obtained for Danuglipron in the corresponding pockets. Notably, Ezetimibe demonstrated a slightly stronger interaction in the C3 pocket than Danuglipron. Overall, Atorvastatin (−8.5 kcal/mol), Fluvastatin (−8.7 kcal/mol), and Rosuvastatin (−8.0 kcal/mol) also showed considerable binding affinities, although their C1 pocket interactions were weaker than those of Danuglipron. Among the nine investigated antihyperlipidemic agents, Pravastatin (−1.2 kcal/mol)

and Simvastatin (−2.2 kcal/mol) displayed the weakest binding affinities. Fenofibrate (−7.9 kcal/mol) and Gemfibrozil (−6.9 kcal/mol) exhibited moderate affinities, whereas Niacin (−5.1 kcal/mol) showed comparatively weaker binding.

Table 1. Calculated binding energies (kcal/mol) of the nine antihyperlipidemic drug and danuglipron

Drug	Binding energy (kcal/mol)			Cavity volume	Center	Docking size
	C1	C2	C3	(C1, C2, C3)	(x,y,z)	(x,y,z)
Atorvastatin	-8,5	-7,7	-8,5	8203, 7987, 3528	114, 129, 86	35,35,24
Pravastatin	-1,2	-9,2	-8,4	8203, 7987, 3529	114, 129, 87	35,35,25
Rosuvastatin	-8,0	-6,9	-8,2	8203, 7987, 3530	114, 129, 88	35,35,26
Simvastatin	-2,2	-10,6	-8,4	8203, 7987, 3531	114, 129, 89	35,35,27
Fluvastatin	-8,7	-7,7	-10,6	8203, 7987, 3532	114, 129, 90	35,35,28
Ezetimibe	-9,0	-8,9	-11,1	8203, 7987, 3533	114, 129, 91	35,35,29
Fenofibrate	-7,9	-8	-10,4	8203, 7987, 3534	114, 129, 92	35,35,30
Gemfibrozil	-6,9	-5,9	-8,6	8203, 7987, 3535	114, 129, 93	35,35,31
Niacin	-5,1	-5,0	-5,1	8203, 7987, 3536	114, 129, 94	35,35,32
Danuglipron	-13,8	-11,4	-9,0	8203, 7987, 3537	114, 129, 95	35,35,33

2.2 Molecular Docking Simulations

The most favorable binding affinities were obtained for Danuglipron, which was used as reference molecule and Ezetimibe with the GLP-1 receptor. Consequently, these ligand–receptor complexes were further analysed using the CB-Dock platform to estimate their binding strengths and interaction profiles with specific amino acid residues [13]. This freely accessible web-based docking tool, which operates through the AutoDock Vina engine, predicts potential binding conformations and corresponding interaction energies. Through this analysis, distinct binding affinities and interaction patterns between the GLP-1 receptor and the investigated ligands were identified.

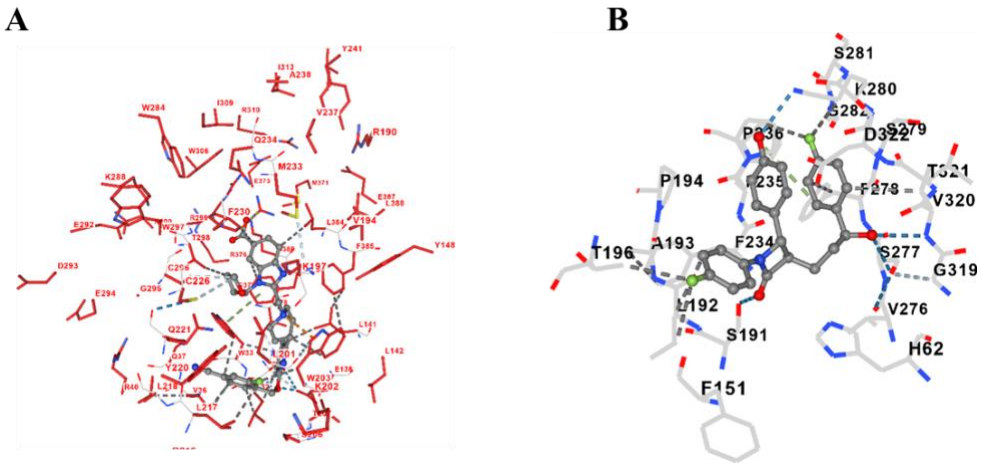


Figure 3. Molecular docking analyses of **A)** Danuglipron **B)** Ezetimibe

Molecular docking analysis revealed that both Ezetimibe and Danuglipron exhibited their most favorable binding affinities within the C1 pocket of the GLP-1 receptor, suggesting that this region constitutes a chemically versatile binding interface. Examination of the amino acid residues involved in ligand–receptor interactions indicated several overlapping physicochemical features rather than identical binding residues.

Ezetimibe primarily interacted with residues located on chain B, including MET61, HIS62, TRP63, CYS148, ARG150, PHE151, and the hydrophobic cluster CYS233–PHE235, forming π–π stacking and hydrogen-bond interactions through its aromatic and hydroxyl moieties (Figure 3). Danuglipron, on the other hand, engaged residues on chain R such as TRP33, GLN37, LEU217, TYR220, PHE230, TRP284, ARG310, and PHE381, within a more deeply buried hydrophobic region enriched in tryptophan and phenylalanine. Despite differences in residue composition, both ligands interacted within an environment rich in aromatic (TRP, PHE), polar (SER, THR, GLN), and positively charged (ARG, LYS) residues, suggesting a shared pattern of π–π stacking, hydrogen bonding, and electrostatic stabilization. The presence of multiple cysteine residues (CYS148, CYS233, CYS317 for Ezetimibe; CYS226, CYS296 for Danuglipron) indicates that both ligands occupy structurally stable regions supported by disulfide linkages (Figure 3). This convergence toward an aromatic–polar–hydrophobic triad of interactions implies that the C1 cavity acts as a general ligand recognition site in GLP-1R. Ezetimibe's relatively superficial engagement, dominated by surface aromatic residues, suggests an allosteric modulatory potential, whereas Danuglipron penetrates deeper into the receptor core, consistent with an agonist-like binding mode capable of inducing conformational activation. Collectively, these findings highlight the chemical complementarity of the C1 pocket and underscore its role as a multifunctional binding region capable of accommodating both canonical GLP-1R agonists and structurally distinct small molecules.

2.3 ADMET Studies

The web base free tool ADMETlab 2.0 was used for determination of toxicological profiles and physicochemical properties of Danuglipron and Ezetimibe (Table 2) [14]. The results show that they have different pharmacokinetic and physicochemical characteristics. Danuglipron is a more polar and heavier molecule (MW: 555.23 Da, TPSA: 113.5 Å²), while Ezetimibe is less polar and smaller. In addition, Ezetimibe exhibits higher drug-likeness (QED: 0.57 vs. 0.311) and better cellular permeability, indicating superior oral absorption. Although both compounds show poor solubility, Ezetimibe has relatively higher solubility. Their lipophilicities are sufficient. According to distribution analysis, both drugs exhibit high plasma protein-binding capacity; however, Ezetimibe has a higher unbound fraction, which may facilitate easier tissue penetration. Metabolic calculations indicate that Danuglipron shows low CYP interactions, whereas Ezetimibe interacts with multiple CYP isoforms. Differences in these metabolic interactions affect clearance rates, with Danuglipron showing a slower elimination rate than Ezetimibe.

Table 2. Physicochemical properties of Danuglipron and Ezetimibe

Category	Property	Danuglipron	Ezetimibe	Interpretation
Physicochemical	Molecular Weight (Da)	555.23	409.15	Danuglipron is heavier and structurally more complex.
Physicochemical	TPSA (Å²)	113.5	60.77	Danuglipron is more polar; Ezetimibe less polar, more permeable.
Physicochemical	logP / logD7.4	3.95 / 3.03	3.32 / 3.24	Both moderately lipophilic; Ezetimibe shows better polarity balance.
Physicochemical	logS (Solubility)	–4.92	–4.26	Both poorly soluble; Danuglipron less soluble.
Physicochemical	nRot / nRig	9 / 34	6 / 23	Danuglipron is more rigid; Ezetimibe more flexible.
Physicochemical	Flexibility Index	0.265	0.261	Both moderately rigid; limited conformational freedom.
Physicochemical	QED (Drug-likeness)	0.311	0.57	Ezetimibe has higher drug-likeness.
Physicochemical	Lipinski Compliance	Accepted	Accepted	Both fulfill major oral drug criteria.
Physicochemical	Pfizer / GSK / Golden Triangle	+ / – / –	– / – / +	Ezetimibe fits Golden Triangle; potentially better absorption.
Absorption	Caco-2 / MDCK (log cm/s)	–5.42 / –4.97	–5.02 / –4.72	Both show moderate-to-low permeability; Ezetimibe slightly higher.
Absorption	logS / logP Relation	Poor solubility, moderate lipophilicity	Slightly better balance	Ezetimibe may have improved oral absorption.
Distribution	Plasma Protein Binding (PPB)	94.1%	90.5%	Both highly bound to plasma proteins; Danuglipron slightly higher.
Distribution	Unbound Fraction (Fu)	4.6%	9.4%	Ezetimibe has higher free fraction → better tissue distribution.
Distribution	Volume of Distribution (VDss, L/kg)	–0.345	0.082	Both mainly confined to plasma compartment.
Metabolism	CYP Inhibition/Substrate Risk	Minimal	CYP2D6, 2C8, 2B6 involvement	Danuglipron shows lower metabolic interaction potential.
Metabolism	Pgp / OATP / MRP / BSEP Interaction	OATP1B3 +++, MRP1 +++, BSEP +++	MRP1 ++, BSEP +++	Both affect hepatic transporters; Danuglipron slightly stronger.
Excretion	Clearance (mL/min/kg)	1.296	5.128	Danuglipron cleared more slowly.
Toxicology	Genotoxicity / Carcinogenicity	0 / 1	1 / 1	Ezetimibe shows higher predicted genotoxic and carcinogenic risk.

3. CONCLUSION

In this study, the GLP-1R binding potential of nine approved antihyperlipidemic drugs through *in silico* docking analyses were performed. Among them, Ezetimibe showed the most comparable binding affinity and interaction profile to Danuglipron, with similar aromatic and polar residues within the C1 pocket of GLP-1R. ADMET analysis revealed that Ezetimibe possesses better drug-likeness, permeability, and solubility. These findings suggest that Ezetimibe may serve as a promising candidate for repurposing as a GLP-1 receptor modulator, warranting further experimental validation.

4. MATERIALS AND METHODS

4.1. Protein and ligand selection

The protein Data Bank (PDB) was used to get the crystal structure of Non peptide agonist PF-06882961, bound to Glucagon-Like peptide-1 (GLP-1) (PDB ID: 6X1A). The SMILE format of the drugs, Atorvastatin, Pravastatin, Rosuvastatin, Simvastatin, Fluvastatin, Ezetimibe, Fenofibrate, Gemfibrozil, Niacin and Danuglipron were downloaded from Drugbank.

4.2. Molecular docking

The Glucagon-Like-peptide-1 (GLP-1) was downloaded as pdb file format. CB-Dock web-based software was used for docking into the active site of the protein. The bindig energies, the size and location of the center were calculated with CB-Dock.

Author contributions: Concept – K.B.; Design – K.B., Ş.K.; Supervision – K.B.; Data Collection and/or Processing – K.B., Ş.K.; Analysis and/or Interpretation – K.B., Ş.K.; Literature Search –K.B.; Writing – K.B., Ş.K.; Critical Reviews – K.B.

Conflict of interest statement: The authors declared no conflict of interest.

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