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Original Article

Bio-Simulation Studies of Valganciclovir Hydrochloride: Molecular Descriptor-Based QSAR Modelling and Swiss ADME Analysis Using *in silico* Models

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ABSTRACT

Aim: To evaluate the pharmacokinetics and toxicity properties of Valganciclovir Hydrochloride, a potent antiviral agent, using *in silico* models. **Background:** Valganciclovir Hydrochloride is an FDA-approved antiviral agent and understanding its pharmacokinetic and toxicological properties is critical for optimizing its use. **Objectives:** To assess the pharmacokinetic properties, toxicity profile and bioactive characteristics of Valganciclovir Hydrochloride using computational *in silico* models. **Materials and Methods:** Lipinski's Rule of Five was applied to evaluate the compound's solubility and intestinal absorption properties. The drug's plasma protein binding and Blood-Brain Barrier (BBB) penetration were also assessed to understand its distribution profile. Clearance rates were calculated to evaluate how efficiently the compound is eliminated from the body. Additionally, the LD_{50} value of Valganciclovir Hydrochloride was estimated using a rat toxicity model to understand its toxicity threshold. Pharmacological activities were further assessed using the PASS online server to evaluate its bioactive properties and potential toxic effects on non-tumor cell lines. **Results:** Valganciclovir Hydrochloride exhibited high solubility and a moderate rate of intestinal absorption. The drug showed low plasma protein binding and poor BBB penetration, suggesting that its distribution is primarily localized within the body. The compound demonstrated a low clearance rate of 5 mL/min/kg. Toxicity analysis revealed an estimated LD_{50} value of 3,080,000 mg/kg via the oral route, indicating a relatively high toxicity threshold. The PASS analysis highlighted various bioactive properties without any toxic effects on non-tumor cell lines, with a Probability of occurrence (Pa) value lower than 0.5, further supporting the non-toxic profile of the compound.

Keywords: *In silico* Modelling, Valganciclovir Hydrochloride, Pharmacokinetics, Toxicity Assessment, Molecular Descriptor, QSAR Modelling.

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INTRODUCTION

An estimated 20 million animals are used annually by the pharmaceutical industry worldwide for *in vivo* studies, which are essential for converting basic biomedical research into discovery and development of new pharmaceuticals or repurposing already-approved medications for novel therapeutic indications.[1,2] However, the ethical concerns, cost and time, associated with animal testing have driven the increasing adoption of *in silico* modelling as a complementary or alternative approach in the early stages of drug development.[3,4]

In silico methods, such as Quantitative Structure-Activity Relationship (QSAR) studies, molecular docking and Absorption-Distribution-Metabolism-Excretion-Toxicity (ADMET) modeling, are increasingly essential in the drug discovery and development process. These computational approaches provide the ability to predict the behavior and properties of drug candidates, significantly reducing reliance on animal models and accelerating the identification of promising compounds.[5] A key principle in the development of New

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Molecular Entities (NMEs) is Lipinski's Rule of Five, which serves as a guideline for "drug-likeness".[6]

According to this rule, a compound is more likely to have poor absorption or permeation if it has more than five hydrogen bond donors, more than ten hydrogen bond acceptors, a molecular weight over 500, or a calculated Log P (CLog P) greater than 5. These guidelines are critical for predicting a compound's pharmacokinetic profile, particularly its absorption and distribution properties.[7,8]

In addition to absorption, the ability of a drug to permeate the skin and cross the Blood-Brain Barrier (BBB) is critical in assessing its potential therapeutic efficacy and safety. A compound with a log Kp value greater than 2.5 is considered to have low skin permeability, while a logBBB (for Blood-Brain Barrier) value greater than - 0.3 indicates a high likelihood of crossing the BBB, which is an important factor in minimizing central nervous system side effects.[9]

Drug metabolism, predominantly mediated by Cytochrome P450 enzymes (CYPs), plays a crucial role in determining the bioavailability and clearance of drug candidates.[10,11] CYPs are involved in over 90% of reported drug metabolism reactions. The excretion rate of a drug, calculated using its clearance rate and half-life, is another vital parameter in understanding its pharmacokinetics.[12] The median Lethal Dose (LD_{50}), which is the dose causing death in 50% of treated animals during acute toxicity testing, remains a standard measure of a compound's acute toxicity.

Valganciclovir, the valine ester prodrug of ganciclovir, represents a significant advancement in antiviral therapy. As the first systemic agent to offer efficacy comparable to intravenous ganciclovir, Valganciclovir has fulfilled a critical need for an oral medication for patients with Cytomegalovirus (CMV) retinitis, particularly during the induction and maintenance phases of therapy.[13,14] In the current research, we aim to establish the pharmacokinetics and toxicity parameters of valganciclovir Hydrochloride using *in silico* models. By leveraging computational tools, this study seeks to provide a detailed understanding of the drug's ADMET properties, potentially guiding further development and optimization for clinical use.

MATERIALS AND METHODS

Lipophilicity

When evaluating lipophilicity, the partition coefficient (log Po/w) between n-octanol and water is a critical indicator. This parameter directly influences the permeability of compounds through biological membranes. A low lipophilicity can hinder permeability, while highly hydrophilic compounds typically lack the ability to passively diffuse across membranes.[15] SwissADME calculates this descriptor using five different models. In our study, we utilized the Consensus log Po/w value to assess the lipophilicity of the molecule.

Solubility

Aqueous solubility is a crucial factor in determining a compound's bioavailability. For a drug to be absorbed, it must first dissolve in water and then possess the ability to permeate biological membranes. In this study, we assessed the bioavailability score. Solubility plays a key role in product development, as it directly impacts bioavailability and serves as an indicator of absorbability.[16] Compounds with poor solubility often require substantial efforts to enhance intestinal absorption during non-clinical phases (such as pharmacokinetic and toxicological studies) and to develop suitable formulations for clinical trials.

Human intestinal absorption

Oral drug administration is the most cost-effective and preferred route, offering high patient compliance. Human Intestinal Absorption (HIA), a critical factor in oral absorption, is one of the most important ADME properties during the early phases of lead discovery and optimization. In this study, HIA was evaluated to predict the absorption behavior of the compounds.[17]

Blood-Brain Barrier

The Blood-Brain Barrier (BBB) is a layer of microvascular endothelial cells that separates the brain from the bloodstream. For drugs targeting the Central Nervous System (CNS), high BBB penetration is essential, while for non-CNS drugs, BBB penetration should be minimized to prevent unwanted side effects. In this study, BBB penetration was assessed to predict the drug's distribution within the brain.[18]

Plasma protein binding

Drugs can bind to plasma proteins at specific rates, which can lead to reduced bioavailability and potential Drug-Drug Interactions (DDI). Therefore, predicting the binding rate is essential to identify and modify problematic drug candidates to improve their safety and effectiveness.[19]

Metabolism

Cytochrome P450 (CYP) enzymes are a family of heme-containing monooxygenases that perform a range of essential functions in the human body. Their primary role is to catalyze the insertion of an oxygen atom into organic molecules while simultaneously reducing a second oxygen atom to form water. In the liver and gastrointestinal tract, these enzymes are key players in phase I metabolism, which involves the biotransformation of both endogenous substances like steroid hormones, lipids and bile acids and exogenous compounds such as drugs, environmental pollutants and dietary phytochemicals. A specific subset of CYP enzymes—namely CYP1A2, CYP2A6, CYP2B6, CYP2Cs (mainly CYP2C9 and CYP2C19), CYP2D6, CYP2E1 and CYP3A4-are

primarily responsible for the metabolism of xenobiotics.[20,21] Among these, certain enzymes take on more significant roles in drug metabolism and the detoxification of foreign substances. Gaining insight into the unique characteristics and activities of these enzymes is essential for accurately predicting metabolic pathways. In this study, we analyzed and evaluated the critical attributes of these CYP enzymes.[22,23]

Toxicity Descriptors

Assessing the toxicity of chemical compounds is essential to identify their potential harmful effects on humans, animals, plants, or the environment. However, *in vivo* animal testing is limited by time constraints, ethical concerns and high costs. As a result, computational approaches are increasingly used to estimate toxicity. *In silico* toxicology serves as a complementary tool to traditional toxicity tests, helping to predict toxicity, prioritize compounds, guide testing strategies and reduce late-stage failures in drug development. In this study, toxicity evaluation was conducted to determine the safety profile of the drug.[24,25]

RESULTS AND DISCUSSION

Physiochemical Properties

The two-dimensional structure of valganciclovir hydrochloride was obtained from PubChem under the ID: 135413534 (Figure 1). The three-dimensional structure was subsequently modeled using Marvin Sketch, followed by energy minimization using the Avogadro software (Figure 2). The conformational analysis identified the most stable 3D conformer of valganciclovir hydrochloride, which was then saved as a PDB file for further analysis and application in the study.

Molecular Weight: The molecular weight of valganciclovir hydrochloride was found 390.82 Daltons (should be less than 500). This criterion helps to ensure that the compound is small enough to be efficiently absorbed in the gastrointestinal tract.

Lipophilicity (LogP): The octanol-water partition coefficient (LogP) was found less than 5. This parameter indicates that the compound is hydrophobic and it can cross cell membranes.

Hydrogen Bond Donors: The number of hydrogen bond donors (counting all nitrogen-hydrogen and oxygen-hydrogen bonds) was found 4 (should be less than 5). This criterion indicates that

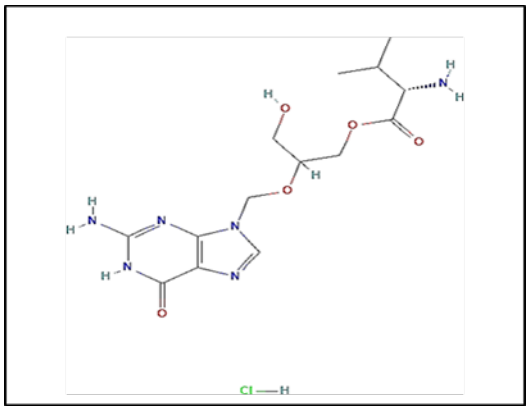

Figure 1: 2D structure of the compound.

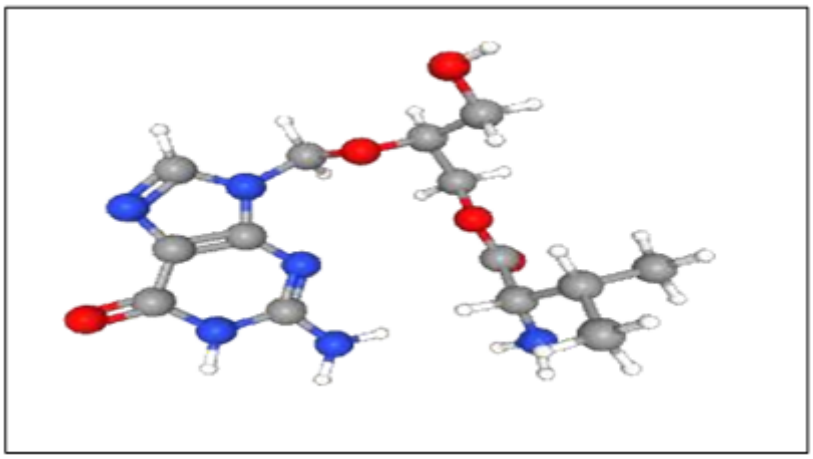

Figure 2: Three-dimensional structure of the compound.

Table 1: Physiochemical Properties.

Formula	Molecular weight	No. of Heavy atom	No. of aromatic heavy atom	No. of Rotatable bond	No. of H- bond Acceptor	No. of H-bond Donor	Total polar surface areaÅ²
$C_{14}H_{23}C_lN_6O_5$	390.82 g/mol	26	9	9	8	4	171.37

Table 2: Solubility and Lipophilicity Properties.

Solubility mg/mL	Class	LogPo/w	Consensus LogPo/w	Lipinski rule of 5	Bioavailability Score
3.63e+00	Soluble	0.00	-0.53	Yes; 1 violation: NorO>10	0.55

Table 3: Results of ADME/T tests.

Properties	Valganciclovir Hydrochloride
ABSORPTION	
Human intestinal absorption	48.560103
Caco-2 permeability	20.8176
LogKp (skin permeation)	-8.56 cm/s
DISTRIBUTION	
P-glyco protein inhibitor	No
Blood-brain barrier penetration	No
Plasma Protein Binding	0.000000
METABOLISM	
CYP3A4 substrate	Weakly
CYP3A4 inhibition	Inhibitor
CYP2C19 inhibition	No
CYP2D6 substrate	Weakly
CYP2D6 inhibition	No
CYP2C9 inhibition	No
EXCRETION	
T1/2 (half-life period)	0.858
Clear ancerate	3.281

the compound is stable enough to form hydrogen bonds with target proteins.

Hydrogen Bond Acceptors: The number of hydrogen bond acceptors (counting all nitrogen and oxygen atoms) was 8 (should not exceed 10). This criterion indicates that the compound is capable enough to interact with target proteins via hydrogen bonding (Tables 1 and 2).

Absorption: High solubility and moderate absorption rate suggest that the valganciclovir hydrochloride could act as a drug in a biological environment. Owing to its very soluble nature and moderate intestinal absorption rate the compound can be used for different routes of administration as a drug (Table 3).

Permeation: Caco-2 permeability is a potential biomarker to determine the oral absorption of any compound. Caco-2 permeability is an important metric in drug discovery and development. Compounds with high Caco-2 permeability are more likely to be absorbed efficiently across the intestinal epithelium, increasing their chances of reaching systemic circulation and exerting their desired pharmacological effects. Here the valganciclovir hydrochloride possesses low Caco2 permeability.

The more negative the log Kp the less skin permeant the molecule. Valganciclovir hydrochloride has a good skin permeation rate.

Distribution: For a compound to be considered a viable drug, it must effectively distribute through systemic circulation. To achieve complete distribution and targeted delivery, the compound must be able to move freely within the circulatory system. P-glycoprotein substrates indicate a compound's ability to penetrate cellular organelles. Valganciclovir hydrochloride, with low plasma protein binding and poor BBB penetration, shows limited interaction with P-glycoprotein, reducing its sedimentation inside cells. Consequently, it primarily exhibits local distribution throughout the body, lowering its potential for widespread therapeutic use.

Metabolism: The metabolic behavior of valganciclovir hydrochloride was predicted using the ADME SIB portal and ADMESAR 2.0 server. Cytochrome P450 (CYP) enzymes, a family of monooxygenases containing heme as a cofactor, are responsible for oxidizing steroids, fatty acids and xenobiotics, playing a key role in chemical clearance and hormone regulation. Valganciclovir hydrochloride inhibits CYP2C19 and CYP2C9, leading to increased plasma concentration. This inhibition can be therapeutically relevant for conditions such as epileptic seizures, candidiasis, bipolar disorder and other psychological disorders, where suppression of these enzymes is beneficial.

Table 4: Results of LD_{50} value of the compound estimated with rat toxicity model.

Rat IP LD_{50} (mg/kg)	Rat IV LD_{50} (mg/kg)	Rat Oral LD_{50} (mg/kg)	Rat SC LD_{50} (mg/kg)
962,900	637,500	3080,000	3211,000

Note: LD_{50}-CLASS; ≤50 - fatal if swallowed (I); 5<LD≤50-fatal if swallowed (II); 50<LD≤300-Toxic if swallowed; 300<LD≤2000-Harmful; 2000 <LD ≤5000 - May be harmful; LD5000 - Non toxic; ECOSAR Test: 10 mg/L - Toxic to environment.

Table 5: Results of LD_{50} value of the compound estimated with ECOSAR test.

Organism	Duration	mg/L(ppm)
Fish	96 hr	1.54e+005
Daphnid	48 hr	66221.367
Green Algae	96 hr	15493.299

Table 6: Environmental toxicity panel with half-life period of the compound.

Models	Half-life period
Half-Life from Model River	2.287E+023 hr
Half-Life from Model Lake	2.495E+024 hr
Air	2.09 hr
Soil	1.8e+003 hr
Sediment	8.1e+003 hr

Table 7: Cytotoxicity of the compound against Normal cell lines.

Pa	Pi	Cell-line	Cell-line full name	Tissue
0.388	0.025	MRC5	Embryonic lung fibroblast	Lung
0.132	0.047	HFF	Foreskin fibroblast	Skin

Clearance: Clearance is a critical pharmacokinetic parameter that, along with the volume of distribution, determines the half-life of a drug and its dosing frequency. Valganciclovir hydrochloride exhibits a clearance rate of 3.8281 mL/min/kg, classified as poor (below the empirical threshold of ≥5 mL/min/kg for excellent clearance). Its half-life is measured at 0.858, which further indicates a poor elimination rate (empirical classification: 0.7-1.0 as poor). Based on the clearance rate and half-life, valganciclovir hydrochloride demonstrates limited elimination efficiency from the body.

Toxicity: Further LD_{50} value of the compounds was estimated using a variety of toxicity models including Rats, Mouse and Fish (Tables 4 and 5).

The compound does not show any kind of toxic effect to non-tumour cell lines. Probability of occurrence (Pa value) lesser than 0.5 clearly proves the nontoxic behaviour of the compound (Tables 6 and 7).

CONCLUSION

The three-dimensional structure of valganciclovir hydrochloride was developed using Marvin Sketch, revealing key insights into its physiochemical properties. The molecular weight of valganciclovir hydrochloride is optimal for gastrointestinal absorption, suggesting its suitability for oral administration. The Log P value indicates that Valganciclovir Hydrochloride is hydrophobic; enabling it to effectively cross cell membranes. The number of hydrogen bond donors in the compound suggests that it is stable and capable of forming hydrogen bonds with target proteins, which is crucial for its interaction and efficacy. Similarly, the number of hydrogen bond acceptors further indicates the compound's potential to engage in hydrogen bonding with target proteins, facilitating its therapeutic action. Valganciclovir Hydrochloride exhibits high solubility and a moderate absorption rate, which are beneficial for its bioavailability. However, the compound shows low plasma protein binding and poor Blood-Brain Barrier (BBB) penetration, suggesting limited distribution within the central nervous system. Analysis of the clearance rate and half-life indicates that valganciclovir hydrochloride has a poor elimination rate, which may impact

its dosing regimen and accumulation in the body. Additionally, the LD_{50} value of the compound was estimated using various toxicity models, including rats, mice and fish. The results show that valganciclovir hydrochloride does not exhibit toxic effects on non-tumor cell lines, further supporting its safety profile.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

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