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Research Article

# Pharmacophore-Based Virtual Screening and Molecular Docking of ZINC Database Compounds Against HIV-1 Integrase

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## ABSTRACT

HIV-1 integrase is a critical enzyme involved in the integration of viral DNA into the host genome and represents an important therapeutic target in antiretroviral drug discovery. In this study, a pharmacophore-based virtual screening approach was carried out using Pharmit, with Dolutegravir as the reference drug. The pharmacophore model included aromatic groups, hydrogen bond donors, hydrogen bond acceptors (4), hydrophobic groups (2), and a negative ionizable feature. A total of 13,127,550 compounds from the ZINC database were screened, and the resulting hits were filtered using Lipinski's Rule of Five, yielding 12 drug-like candidate molecules. Molecular docking was subsequently performed against HIV-1 integrase (PDB ID:3S3M) using AutoDock Vina. Among the screened compounds, ZINC000299738148 and ZINC000299738315 emerged as the top lead candidates, with binding energies of −9.7 kcal/mol and −9.4 kcal/mol, respectively. Notably, ZINC000299738148 exhibited a stronger binding affinity than the reference drug Dolutegravir (−9.5 kcal/mol), while ZINC000299738315 showed comparable binding performance. Both lead compounds demonstrated stable interactions with key active site residues, including ARG350, GLN215, HIS213, and SER216, similar to Dolutegravir, indicating a conserved binding mode. These findings suggest that the identified compounds may serve as promising inhibitors of HIV-1 integrase and warrant further investigation.

## 1. Introduction

Human Immunodeficiency Virus (HIV) remains a major global health concern, with approximately 39.9 to 40.8 million people affected worldwide (UNAIDS 2020; WHO 2024). The virus attacks the immune system, specifically CD4+ T cells, leading to progressive immune failure and increased susceptibility to opportunistic infections (Abbas et al.,2023) Despite significant advances in antiretroviral therapy (ART), the emergence of drug resistance particularly to newer integrase inhibitors and long-term metabolic toxicities continue to challenge effective disease management (Eron et al., 2023; Gandhi et al.,2025). Therefore, the discovery of novel therapeutic agents with improved genetic barriers to resistance and superior safety profiles remains a critical need for global epidemic control, (WHO,2022; Quashie et al.,2012).

HIV-1 integrase is a key enzyme responsible for the integration of viral DNA into the host genome, an essential step in the viral replication cycle (Mbhele et al., 2021) Due to its crucial role, integrase has become an attractive target for drug development (Mbhele et al.,2021; Li et al.,2012) Clinically approved integrase strand transfer inhibitors (INSTIs), such as Dolutegravir, have shown high potency and a favourable resistance profile (Li et al.,2012). However, resistance mutations and variability in patient response necessitate the identification of new inhibitors with enhanced binding characteristics and reduced side effects (Li et al.,2012; Lionta et al., 2014)

In recent years, computational approaches such as pharmacophore modeling, virtual screening, and molecular docking have significantly accelerated the drug discovery process (Yang, 2010; Irwin et al., 2005) Pharmacophore-based screening allows the identification of compounds with essential chemical features required for biological activity, while virtual screening enables rapid evaluation of large chemical libraries (Yang, 2010; Irwin et al., 2005). Databases such as ZINC database provide access to millions of purchasable compounds, facilitating large-scale screening efforts (Lipinski et al.,1997). Additionally, Lipinski's Rule of Five is widely used to filter compounds for drug-likeness, improving the probability of identifying orally active candidates (Sunseri et al., 2006).

In this study, a pharmacophore-based virtual screening approach was employed using Pharmit, taking Dolutegravir as the reference compound (Trott et al., 2010) Key pharmacophore features were defined and used to screen over 13 million compounds from the ZINC database, followed by Lipinski's Rule of Five filtering to obtain drug-like candidates (Lipinski et al., 1997; Sunseri et al., 2006)

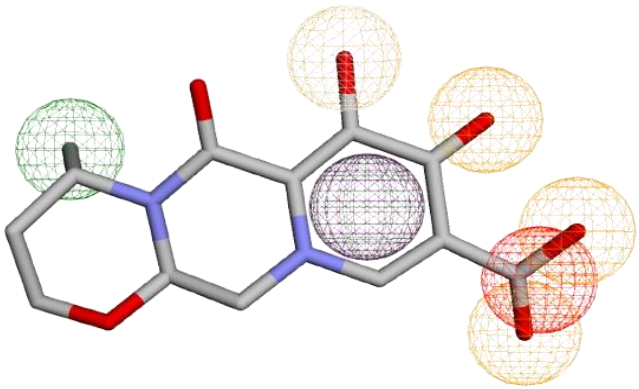
The selected compounds were then subjected to molecular docking against HIV-1 integrase (PDB ID: 3S3M) using AutoDock Vina (Trott et al., 2006) The objective of this study is to identify potential lead compounds with strong binding affinity and favorable interaction profiles that may serve as promising HIV-1 integrase inhibitors.

## 2. Materials and Methods

### *2.1. Pharmacophore Model Generation*

A pharmacophore-based virtual screening approach was employed using the Pharmit online server (Sunseri et al., 2016) The three-dimensional structure of the reference drug, Dolutegravir, was used to generate the pharmacophore model (Canduci,2011). Essential chemical features responsible for biological activity were identified and selected, including aromatic rings, hydrogen bond donors (HBD), hydrogen bond acceptors (HBA = 4), hydrophobic groups, and a negative ionizable feature, consistent with standard pharmacophore modeling principles (Sunseri et al., 2016; Yang, 2010). These features were spatially arranged to define the pharmacophore query for screening.

**Fig.1** Pharmacophore models based on the Crystal Structure of the CCR5 integrase enzyme Receptor with Doultegravir (PDB ID: 3S3M) and generated with pharmit server



### *2.2. Virtual Screening of ZINC database*

The generated pharmacophore model was used to screen compounds from the ZINC database, a large repository of commercially available chemical compounds (Irwin et al., 2005). A total of 13,127,550 molecules were screened based on the defined pharmacophore constraints. To ensure drug-likeness, the resulting hits were further filtered using Lipinski's Rule of Five, which evaluates molecular properties such as molecular weight, lipophilicity (LogP), hydrogen bond donors, and hydrogen bond acceptors (Lipinski et al., 1997) After filtering, 12 compounds were selected as potential candidates for further analysis.

### *3. Drug-Likeness Prediction*

The drug-likeness properties of the selected compounds were evaluated using the SwissADME web server (Daina et al., 2017). This tool provides a comprehensive assessment of pharmacokinetic and physicochemical properties, enabling the identification of compounds with favorable oral bioavailability (Daina et al., 2017). The screened ligands, along with the reference drug Dolutegravir, were subjected to multiple drug-likeness filters, including Lipinski's Rule of Five (Lipinski et al.,1997) the Ghose filter (Ghose et al.,1999) the Veber rule (Veber et al., 2002) the Egan rule (Egan et al., 2000) and the Muegge filter (Muegge et al., 2001).

Lipinski's Rule of Five was used to evaluate molecular weight, lipophilicity (LogP), hydrogen bond donors, and hydrogen bond acceptors to determine oral drug-likeness (Lipinski et al.,1997). The Ghose filter assessed parameters such as molar refractivity and atom count (Ghose et al.,1999), while the Veber rule focused on rotatable bonds and topological polar surface area (TPSA) (Veber et al., 2002). The Egan rule evaluated absorption properties (Egan et al., 2000), and the Muegge filter provided an additional layer of drug-likeness validation (Muegge et al., 2001).Compounds satisfying these criteria are considered to possess favorable pharmacokinetic profiles and higher potential for oral bioavailability. The drug-likeness evaluation revealed that the majority of the screened compounds exhibited favorable pharmacokinetic properties. All selected ligands, including the reference drug Dolutegravir, successfully passed Lipinski's Rule of Five, indicating good oral drug-likeness and compliance with essential physicochemical parameters.

Further analysis using additional filters showed that most compounds satisfied the Ghose, Veber, Egan, and Muegge criteria, suggesting overall favorable absorption, distribution, and permeability characteristics. Notably, compounds such as ZINC000000008750, ZINC000035342789, ZINC000035645588, ZINC000036384898, ZINC000070453768, ZINC000095975444, ZINC000096288818, ZINC000104211987, ZINC000299738148, and ZINC000299738315 passed all evaluated filters, indicating excellent drug-likeness profiles.

However, a few compounds showed minor deviations. ZINC000004016753 failed the Muegge filter, ZINC000104211987 showed a violation in the Egan rule, and ZINC000113072889 failed the Ghose filter. Despite these minor violations, these compounds still satisfied Lipinski's criteria and most other filters, suggesting that they may retain acceptable pharmacokinetic properties.

Importantly, the top lead compounds ZINC000299738148 and ZINC000299738315 passed all drug-likeness filters without any violations, similar to Dolutegravir. This indicates that these compounds not only exhibit strong binding affinity but also possess favorable physicochemical and pharmacokinetic characteristics, enhancing their potential as promising drug candidates

The SwissADME analysis confirms that the majority of the screened compounds have suitable drug-like properties, supporting their further evaluation in drug development pipelines.

### *3.2 Ligand Preparation*

The selected hit compounds were obtained from the ZINC database in SDF format. These structures were converted into PDBQT format using AutoDock Tools to make them compatible

**Table 1.** Drug-Likeness Results

| s.no | Ligand | Lipinski violations | Ghose violations | Veber violations | Egan violations | Muegge violations |
|---|---|---|---|---|---|---|
| 1. | ZINC000000008750 | Pass | Pass | Pass | Pass | Pass |
| 2. | ZINC000004016753 | Pass | Pass | Pass | Pass | Fail |
| 3. | ZINC000035342789 | Pass | Pass | Pass | Pass | Pass |
| 4. | ZINC000035645588 | Pass | Pass | Pass | Pass | Pass |
| 5. | ZINC000036384898 | Pass | Pass | Pass | Pass | Pass |
| 6. | ZINC000070453768 | Pass | Pass | Pass | Pass | Pass |
| 7. | ZINC000095975444 | Pass | Pass | Pass | Pass | Pass |
| 8. | ZINC000096288818 | Pass | Pass | Pass | Pass | Pass |
| 9. | ZINC000104211987 | Pass | Pass | Pass | Fail | Pass |
| 10. | ZINC000113072889 | Pass | Fail | Pass | Pass | Pass |
| 11. | ZINC000299738148 | Pass | Pass | Pass | Pass | Pass |
| 12. | ZINC000299738315 | Pass | Pass | Pass | Pass | Pass |
| 13. | Dolutegravir | Pass | Pass | Pass | Pass | Pass |

with docking simulations. During preparation, polar hydrogens were added, and Gasteiger charges were assigned to each ligand. Rotatable bonds were defined to allow flexible dockin (Irwin et al., 2005; Kumar Thatipamula et al., 2017).

### *3.3 Protein Preparation*

The crystal structure of HIV-1 integrase (PDB ID: 3S3M) was retrieved from the Protein Data Bank. Protein preparation was carried out using BIOVIA Discovery Studio and AutoDock Tools. Water molecules and co-crystallized ligands were removed, and missing hydrogen atoms were added. Kollman charges were assigned, and the protein structure was converted into PDBQT format for docking studies (Morris et al., 2009; Trott et al., 2010; Porika et al., 2014; Poojari et al., 2014).

### *3.4 Grid Box Generation*

A grid box was defined around the active site of the HIV-1 integrase enzyme to ensure proper ligand binding during docking. The grid parameters, including center of a grid box size 120 × 120 × 120 Å with grid point's level x =-48.71, y =33.895, and z = -23.474 with partial charge cut-off (0.25 Å) was predicted with centroid co-crystallized ligand by applying force field coordinates and dimensions, were set based on the position of the co-crystallized ligand and key active site residues. This step was performed using AutoDock Tools.

### *3.5 Molecular Docking*

Molecular docking studies were conducted using AutoDock Vina to evaluate the binding affinity of the selected compounds with HIV-1 integrase (Hare et al., 2010; Mamidala et al., 2020). All 12 screened ligands, along with the reference drug Dolutegravir, were docked into the active site of the protein. Default docking parameters were used, and binding affinity was measured in terms of binding Hydrogen bonding plays a crucial role in stabilizing ligand–protein interactions and contributes significantly to binding affinity. In the present study, the number of hydrogen bonds formed between the ligands and the protein ranged from 3 to 5, indicating strong and stable interactions within the active site. Compounds such as ZINC000004016753, ZINC000035645588, and ZINC000036384898 formed up to five hydrogen bonds, suggesting enhanced binding stability. The top-ranked compound, ZINC000299738148, formed four hydrogen bonds with key residues including SER216, ARG350, THR351, and SER365, which are essential for integrase activity. Similarly, ZINC000299738315 formed hydrogen bonds with HIS213, GLN215, and ARG350, closely resembling the interaction pattern observed with the reference drug Dolutegravir. The best docking poses were selected based on the lowest binding energy values.

## 4. Results and Discussion

### *4.1 Molecular Docking Analysis*

The pharmacophore-based virtual screening followed by Lipinski filtering resulted in 12 potential lead compounds, which were further subjected to molecular docking against HIV-1 integrase (PDB ID: 3S3M) using AutoDock Vina. The docking results were evaluated based on binding energy (kcal/mol), number of hydrogen bonds, and interaction with key active site residues. Among all screened compounds, binding energies ranged from −6.7 to −9.7 kcal/mol, indicating favorable interactions within the active site of HIV-1 integrase. Notably, most compounds exhibited strong binding affinities comparable to or better than the reference drug Dolutegravir.

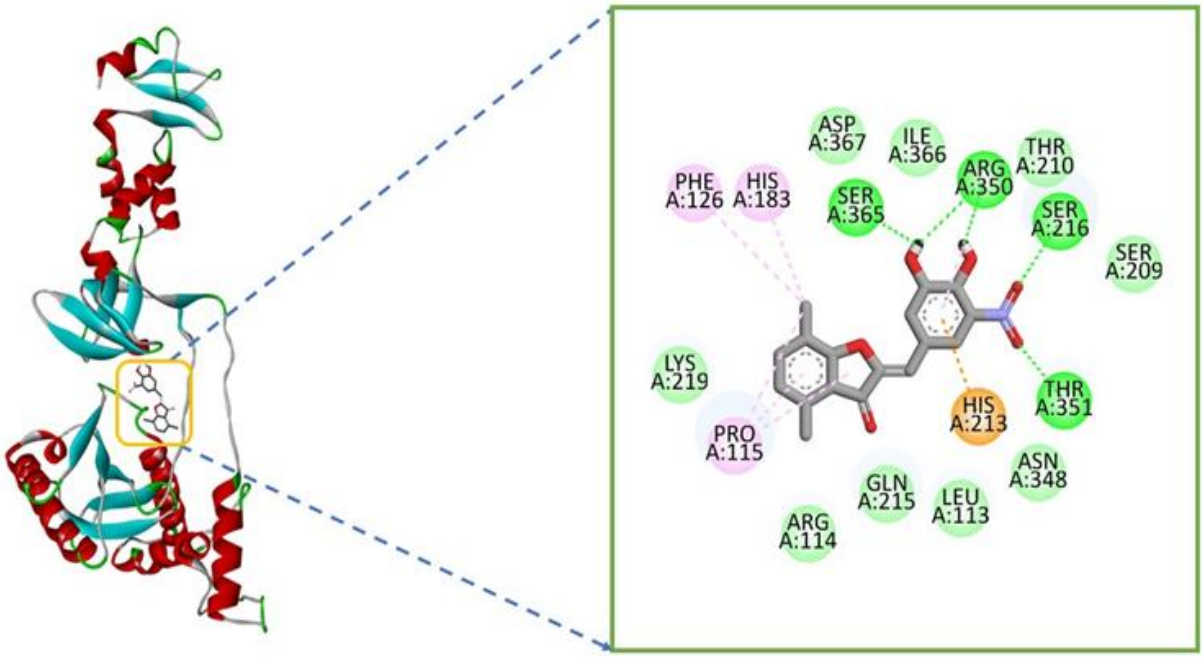
### *4.2 Identification of Top Lead Compounds*

The molecular docking results revealed that among all the screened compounds, ZINC000299738148 and ZINC000299738315 emerged as the top-performing lead molecules with binding energies of −9.7 kcal/mol and −9.4 kcal/mol, respectively. Notably, ZINC000299738148 exhibited the highest binding affinity, surpassing the reference drug Dolutegravir (−9.5 kcal/mol), indicating a stronger and more stable interaction with the active site of HIV-1 integrase. Similarly, ZINC000299738315 demonstrated a binding energy very close to that of Dolutegravir, suggesting comparable inhibitory potential. In addition to these top candidates, other compounds such as ZINC000035342789 and ZINC000036384898 also showed favorable binding affinities (−8.6 kcal/mol), indicating that multiple screened ligands possess promising activity against the target protein. Detailed analysis of ligand–protein interactions revealed that several amino acid residues consistently participated in binding across all docked compounds. The core active site residues stabilization and enzymatic inhibition. In addition, hydrophobic interactions were observed with residues such as

**Table 2**. Molecular docking analysis of retrieved compounds against Integrase receptor protein (PDB: 3SM3)

| S.No | Ligand | B.E (kcal/mol) | H bonds | Hydrogen bond interactive AAs | Other interactions |
|---|---|---|---|---|---|
| 1. | ZINC000000008750 | -8.4 | 3 | Leu113, Gln215, Arg350 | Ile112, Leu113, Phe126, His183, His213, Ser216, Thr210, Asn348, Ser365 |
| 2. | ZINC000004016753 | -8.5 | 5 | Arg113, Arg114, Ser216, Lys219, Arg350 | Ile112, Pro115, Gly218, Phe126his213gln215, Ser217, Asn358, Thr351, Ser365, Ile366 |
| 3. | ZINC000035342789 | -8.6 | 4 | Thr210, Ser216, Arg350, Thr351 | Ile112, Leu113,Pro115,Ser209, His213, Gln215, Asn348,Val364,Ser365,Ile366,Asp367 |
| 4. | ZINC000035645588 | -7.5 | 5 | Leu113, Gln215, Asn348, Arg350, Thr351 | Ile112,Leu113,Pro115,Ser209,His213, Gln215, Asn348,Val364,Ser365, Ile366,Asp367 |
| 5. | ZINC000036384898 | -8.6 | 5 | Leu113, Thr210, Ser216, Arg350, Thr351 | Ile112,Pro115,Ser209,His213, Gln215,Asn348, ,Ser365,Ile365,Asp367 |
| 6. | ZINC000070453768 | -7.3 | 3 | Leu113, Gln215, Arg350 | Ile112pro115,Arg114,His213,Gly218 |
| 7. | ZINC000095975444 | -6.7 | 4 | Leu113, Arg114, Gln215, Arg350 | Ile112pro115,Phe126 ,His213,Ser216,Gly218 |
| 8. | ZINC000096288818 | -8 | 4 | Leu113, Gln215, Ser216, Gln215 | Ile112pro115,Phe126, His213,Ser217,Gly218,Lys219 |
| 9. | ZINC000104211987 | -7.9 | 3 | Leu113, Gln215, Arg350 | Ile112,Arg114,Pro115, Lts124,Phe126,His184,Gly218ser216 |
| 10. | ZINC000113072889 | -8.4 | 3 | His213, Gln215, Arg350 | Ile112,Arg114,Pro115leu113,Phe126, Gly218,Lys219,Thr210,Asn348,Thr351,Ser365 |
| 11. | ZINC000299738148 | -9.7 | 4 | Ser216, Arg350, Thr351, Ser365 | Leu113, Arg114, Pro115, Phe126, His183, Ser209, Thr210, His213, Asn348, Ile366, Asp367 |
| 12. | ZINC000299738315 | -9.4 | 3 | His213, Gln215, Arg350 | Ile112, Arg114, Pro115, Phe126leu113, Thr210, Gly218, Lys219, Asn348, Thr351, Ser365 |
| 13. | Dolutegravir (Reference Drug) | 9.5 | 4 | Arg114, Gln215, His213, Thr21o | Ile112, Leu113, Pro115, Ser216, Lys219, Gly218, Asn348, Arg350, Thr351, Ser365 |

**Fig. 2** 3D and 2D visualization of molecular docking results of ZINC000299738148



ILE112, LEU113, PRO115, and PHE126, further contributing to binding stability. The repeated involvement of these residues across multiple ligands suggests that the screened compounds occupy the same binding pocket as Dolutegravir and follow a similar binding mechanism involved in interactions include significant role in ligand.

The reference drug Dolutegravir exhibited a binding energy of −9.5 kcal/mol with four hydrogen bonds, interacting with key residues such as ARG114, GLN215, HIS213, and THR210. In comparison, ZINC000299738148 demonstrated a superior binding affinity (−9.7 kcal/mol) along with strong interactions involving critical residues, indicating its potential as a more effective inhibitor than Dolutegravir. On the other hand, ZINC000299738315 showed comparable binding energy (−9.4 kcal/mol) and similar interaction patterns, suggesting that it may serve as an alternative inhibitor. Furthermore, many of the screened compounds shared common interaction residues with Dolutegravir, particularly GLN215, HIS213, ARG350, and SER216, which validates the effectiveness and reliability of the pharmacophore model used in this study. (Hare et al., 2010; Li et al., 2023; Lunavath et al, 2015; Kumar et al., 2020).

## 5. Conclusion

In the present study, a pharmacophore-based virtual screening approach combined with molecular docking was successfully employed to identify potential inhibitors of HIV-1 integrase. A pharmacophore model generated using Dolutegravir as the reference compound was used to screen 13,127,550 compounds from the ZINC database. Following the application of Lipinski's Rule of Five, 12 drug-like compounds were selected and subjected to molecular docking analysis against HIV-1 integrase (PDB ID: 3S3M). The docking results revealed that several screened compounds exhibited strong binding affinity toward the active site of the enzyme. Notably, ZINC000299738148 demonstrated the highest binding affinity (−9.7 kcal/mol), surpassing the reference drug Dolutegravir (−9.5 kcal/mol), while ZINC000299738315 showed comparable binding energy (−9.4 kcal/mol). Both compounds formed stable hydrogen bond interactions with key active site residues such as ARG350, GLN215, HIS213, and SER216, indicating a conserved binding mode similar to that of Dolutegravir.

## Competing interests:

The authors declare that they have no competing interests

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