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# *In-Silico* Molecular Docking Studies of Crinum Solapurense: For Cox-Inhibition

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**Abstract**

In the present study, an aim was to identify adrug-likecandidate for the plant *Crinum Solapurense*(Amaryllidaceae).The Lycorine, an alkaloid that could be a potential candidate which can interact and inhibits the cyclooxygenase-2 (COX-2) generated protein 5KIR and relieves pain and inflammation.Total 18 compounds were analyzed through, Autodock vina. The docking value was observed in the range of -9.4 to −10.3 kcal·mol$^{-1}$. No other article and review have been reported for the molecular docking study for the plant *Crinum Solapurense.*Moreover, there have been some articles of plants belonging to the family Amaryllidaceae.

**Key words:** *Crinum Solapurense,* Amaryllidaceae, AutoDock Vina, Lycorine, cyclooxygenase-2 etc.

## Introduction

The Solapur district is largely an agricultural land gifted with a variety of natural resources in the plains of Bhima, Sina and Man Rivers. The grasslands of district are unique and popularly famous for bird diversity. The Indian Bastard inhabits in these grasslands.125 families of flowering plants are available in the Solapur district. Majorly Fabaceae, Poaceae, Euphorbiaceae, Apocynaceae, Solanaceae and Amaryllidaceae families are reported in taxonomic work. The Amaryllidaceae is a large family of monocotyledonous, bulbous flowering plants of ground. It is widely distributed from temperate to tropical region. It contains about 90 genera and 1310 species.(1)The specific Alkaloids produced by this plant have attracted attention of researchers and they have interesting pharmacological activities. The plants from Amaryllidaceae family are useful in drug development. In Maharashtra, the plant is available in bordering the Bhima river between Machnur village in Solapur district and in western ghats named *Crinum Solapurense*. In India detailed work on Crinum is carried out by William Roxburghe flora, he reported 14 species from British India. (2, 3)

*CrinumSolapurense*traditionally cultivated or ornamental due to large conspicuous, beautifulumbels of lily like flower, but they have known to be medicinal herbs. Flowers leaves sliced orcrushed bulbs and stalks of these plants have been used for centuries to cure aliments and diseases due to their medicinal properties; due to this it attracted the attention of the general public, plant gathers, herbalists and medicinal science researchers.(4)

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Fig: 1 *Crinum Solapurense* Plant

Different biological investigation was carried out on various varieties of Crinum species, the total extract was taken and bioactive compounds were isolated and it shows wide pharmacological effects such as analgesic, anti-inflammatory, antinociceptive and anti-Alzheimer activity. *C giganteum* bulbs and *C. glaucum* bulbs shown significant analgesic and anti-inflammatory effect.(5, 6, 7) The two major alkaloids which found in Amaryllidaceae plants are Lycorine and Galantamine (6).

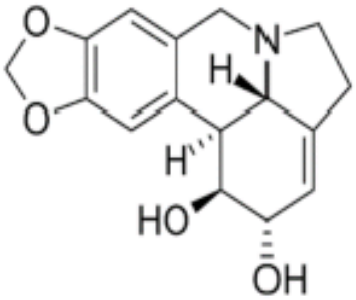



Fig 2: Structure of Lycorine

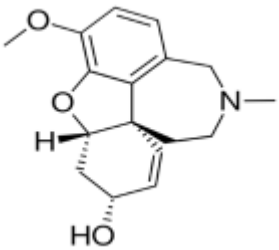



Fig 3: Structure of Galantamine

## Materials and methods (7, 8, 9)

### *Molecular docking*

### *Ligand and protein preparation*

A) *Ligand structure retrieval*

Ligand structures drawn using King-Draw. And Structures were saved in MOL or SDF format

B) *Conversion to 3D structure*

2D ligands were converted into 3D conformations and Geometry was checked for proper bond angles and stereochemistry.

C) *Energy Minimization of Ligands*

Ligands were energy-minimized using:Open Babel (MMFF94 force field) or Avogadro. The lowest energy conformer was selected.

D) *Protonation and Charge Assignment*

Gasteiger charges were added to ligands.All hydrogens were added.Rotatable bonds were defined.

E) *Ligand File Preparation*

Ligands were saved in .pdbqt format using Autodock Tools.Torsional degrees of freedom were verified.

All the input files for docking were prepared using graphical user interface of Biovia Discovery Studio Visualizer and MGLTools packages. Molecular interaction of HS-01 with numerous anti-inflammatory drug targets was studied by molecular docking using two different programs namely, AutoDock 4.2 and AutoDock Vina 1.1. Native co-crystalized ligands, water molecules and cofactors were removed from each PDB file and Gasteiger method was used for assigning partial atomic charges. Each rotatable bond of ligand was assigned after merging non-polar hydrogens. A grid box having dimension of 60, 60, and 60 points in x, y, and z directions was built with grid spacing of 0.375 Å. Distance-dependent function of the dielectric constant was used for the calculation of the energetic map. The default settings were used for all other parameters. Upon completion of docking, the best poses were screened by exam-

ination of binding energy (ΔGbinding, kcal/mol) and number in cluster. Molecular interactions of both hydrophobic and hydrophilic types and root mean square deviation (RMSD) were studied using Biovia Discovery Studio Visualizer6.

In the present study, shown the number of macromolecular targets associated with inflammatory cascade such as cyclooxygenase-2 (COX-2)

Prior to the docking of test compound, all co-crystallized ligands were redocked into their respective proteins (PDB ID: 5KIR)

***In-silico ADME prediction***

Using the SwissADME web-based tool, computational analyses of the shortlisted compounds (18 compounds) were carried out in order to predict their molecular features.

Molecular features relating to the pharmacokinetics such as, ADME profile, bioavailability, drug-likeliness and medicinal chemistry properties of the synthesized compounds were assessed. Input of each compound was provided to the simulations tool in the form of Canonical SMILES. In order to predict drug-likeness, the tool estimates bioavailability radar based on six physicochemical attributes, comprising of lipophilicity, size, polarity, solubility, flexibility, and saturation.

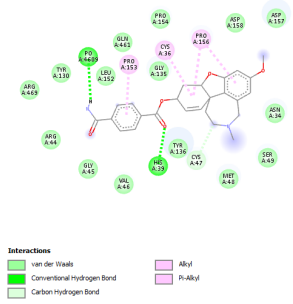
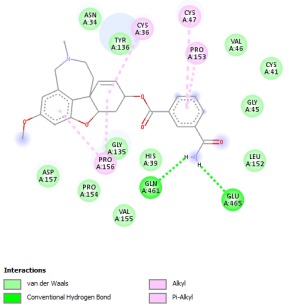
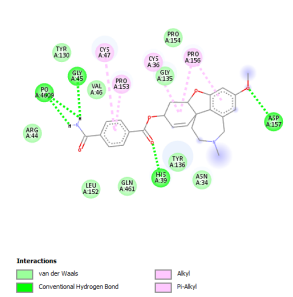
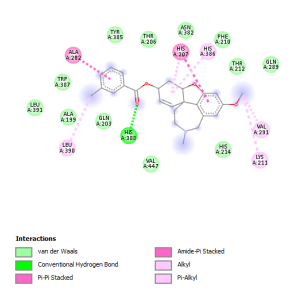
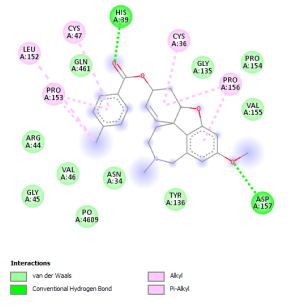
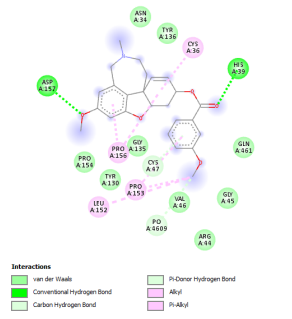
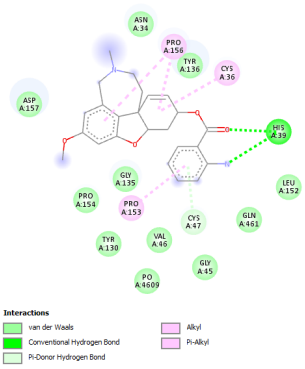
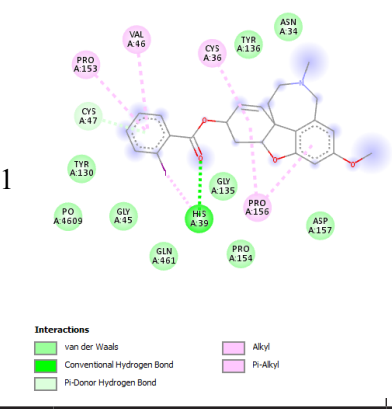
The ADME features, namely blood-brain barrier (BBB) penetration and passive human gastrointestinal absorption (HIA), as well as substrate or non-substrate of the permeability glycoprotein (P-gp), as observed to be positive or negative in the BOILED-Egg model. According to the generalized-born and solvent accessible surface area (GB/SA) model created by (18), the estimation of lipophilicity (Log p/w) parameters such as iLOGP was determined for n-octanol and water on free energies of solvation. (19) created the atomistic technique known as XLOGP3, which includes correction elements and a knowledge-based library. WLOGP has been built for a completely atomistic technique based on the (20) fragment system. According to researchers, M-LOGP is an example of a topological technique and relies on a linear connection with 13 molecular descriptors, whereas SILICOS-IT is a hybrid method that relies on 27 fragments and 7 topological descriptors (21).

The rule-of-five pioneer Lipinski (Pfizer) filter has been implemented into this tool from (23), and this tool also includes an inbuilt feature for the prediction of drug-likeness (21). SwissADME tool has created the bioavailability radar for oral bioavailability prediction according to several physico-chemical factors (21). The Lilly MedChem (24) filters applied to clean chemical libraries of compounds most likely unstable, reactive, toxic, or prone to interfere with biological assays because unspecific frequent hitters, dyes, or aggregators (25), PAINS structural alert, or pan assay interference compounds (26), have all been used to predict medicinal chemistry techniques (27). The synthetic accessibility (SA) score is essentially based on the supposition that the frequency of molecular fragments in'really' attainable compounds corresponds with the simplicity of synthesis. The created and verified technique has been presented by (28) using the molecule synthetic accessibility score, which ranges from 1 to 10 (easy and extremely difficult to synthesize).

**Results and Discussion**

Table 1: Docking studies of the compounds with 5KIR protein

| Target Compounds | Interacting structure with protein | Docking value (Affinity kcal/mol) |
|---|---|---|

| | | |
|---|---|---|
| 17 |  | -9.8 |
| 23 |  | -10.1 |
| 24 |  | -10.0 |
| 26 |  | -10.3 |
| 27 |  | -9.5 |
| 30 |  | -9.5 |
| 31 |  | -9.4 |
| 41 |  | -9.5 |

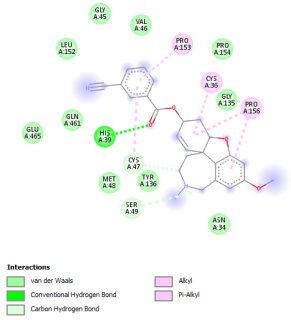
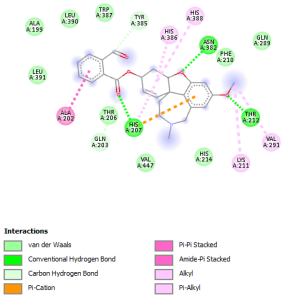
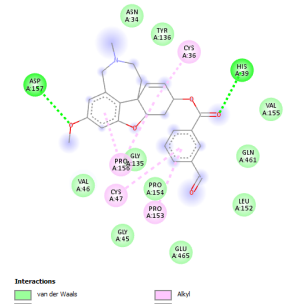
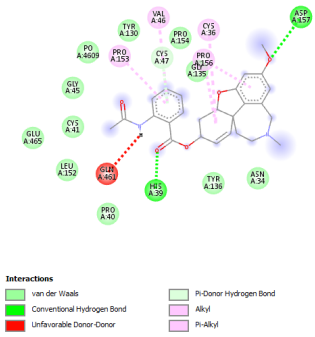
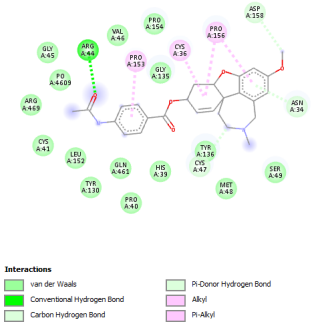
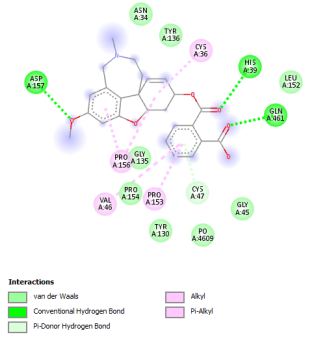
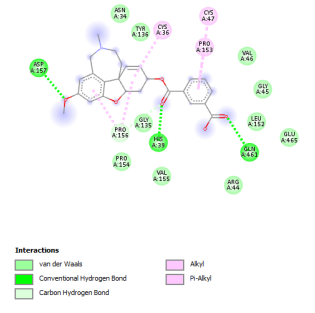
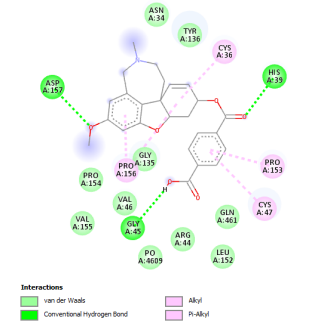
| | | |
|---|---|---|
| 54 |  | -9.5 |
| 56 |  | -9.4 |
| 57 |  | -9.4 |
| 59 |  | -9.9 |
| 61 |  | -9.7 |
| 62 |  | -9.6 |
| 63 |  | -9.5 |
| 64 |  | -10.0 |

Table 2: Canonical SMILES and Physicochemical properties of shortlisted compounds

| Sr | Compound | Canonical SMILES | Molecular formula | Molecular weight ($g \cdot mol^{-1}$) | Rotatable bonds (n) | H-bond acceptors (n) | H-bond donors (n) | TPSA ($Å^2$) |
|---|---|---|---|---|---|---|---|---|
| 1 | 17 | COC1=CC2=C3[C@]4([C@@]([C@@H](OC(C5=CC=C(C(N)=O)C=C5)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{25}H_{26}N_2O_5$ | 434.48 | 5 | 6 | 1 | 91.09 |
| 2 | 23 | COC1=CC2=C3[C@]4([C@@]([C@@H](OC(C5=CC=CC(C(N)=O)=C5)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{25}H_{26}N_2O_5$ | 434.48 | 5 | 6 | 1 | 91.09 |
| 3 | 24 | COC1=CC2=C3[C@]4([C@@]([C@@H](OC(C5=CC=C(C(N)=O)C=C5)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{25}H_{26}N_2O_5$ | 434.48 | 5 | 6 | 1 | 91.09 |
| 4 | 26 | COC1=CC2=C3[C@]4([C@@]([C@@H](OC(C5=CC=CC(C)=C5)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{25}H_{27}NO_4$ | 405.49 | 4 | 5 | 0 | 48 |
| 5 | 27 | COC1=CC2=C3[C@]4([C@@]([C@@H](OC(C5=CC=C(C)C=C5)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{25}H_{27}NO_4$ | 405.49 | 4 | 5 | 0 | 48 |
| 6 | 30 | COC1=CC2=C3[C@]4([C@@]([C@@H](OC(C5=CC=CC(OC)=C5)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{25}H_{27}NO_5$ | 421.49 | 5 | 6 | 0 | 57.23 |
| 7 | 31 | COC1=CC2=C3[C@]4([C@@]([C@@H](OC(C5=CC=CC=C5N)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{24}H_{26}N_2O_4$ | 406.47 | 4 | 5 | 1 | 74.02 |
| 8 | 41 | COC1=CC2=C3[C@]4([C@@]([C@@H](OC(C5=CC=CC=C5I)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{24}H_{24}INO_4$ | 517.36 | 4 | 5 | 0 | 48 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 9 | 43 | COC1=CC2=C3[C@]4([C@@][C][C@@H](OC(C5=CC=C(I)C=C5)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{24}H_{24}INO_4$ | 517.36 | 4 | 5 | 0 | 48 |
| 10 | 51 | COC1=CC2=C3[C@]4([C@@][C][C@@H](OC(C5=CC=CC(S(=O)(O)=O)=C5)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{25}^{24}H_{25}NO_7S$ | 471.52 | 5 | 8 | 1 | 110.75 |
| 11 | 54 | COC1=CC2=C3[C@]4([C@@][C][C@@H](OC(C5=CC=CC(C#N)=C5)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{25}H_{24}N_2O_4$ | 416.47 | 4 | 6 | 0 | 71.79 |
| 12 | 56 | COC1=CC2=C3[C@]4([C@@][C][C@@H](OC(C5=CC=CC=C5C([H])=O)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{25}H_{25}NO_5$ | 419.47 | 5 | 6 | 0 | 65.07 |
| 13 | 57 | COC1=CC2=C3[C@]4([C@@][C][C@@H](OC(C5=CC=CC(C([H])=O)=C5)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{25}H_{25}NO_5$ | 419.47 | 5 | 6 | 0 | 65.07 |
| 14 | 59 | COC1=CC2=C3[C@]4([C@@][C][C@@H](OC(C5=CC=CC=C5NC(C)=O)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{26}H_{28}N_2O_5$ | 448.51 | 6 | 6 | 1 | 77.1 |
| 15 | 61 | COC1=CC2=C3[C@]4([C@@][C][C@@H](OC(C5=CC=C(NC(C)=O)C=C5)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{26}H_{28}N_2O_5$ | 448.51 | 6 | 6 | 1 | 77.1 |
| 16 | 62 | COC1=CC2=C3[C@]4([C@@][C][C@@H](OC(C5=CC=CC=C5C(O)=O)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{25}H_{25}NO_6$ | 435.47 | 5 | 7 | 1 | 85.3 |
| 17 | 63 | COC1=CC2=C3[C@]4([C@@][C][C@@H](OC(C5=CC=CC(C(O)=O)=C5)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{25}H_{25}NO_6$ | 435.47 | 5 | 7 | 1 | 85.3 |
| 18 | 64 | COC1=CC2=C3[C@]4([C@@][C][C@@H](OC(C5=CC=C(C(O)=O)C=C5)=O)C=C4)([H])OC3=C1)CCN(C)C2 | $C_{25}H_{25}NO_6$ | 435.47 | 5 | 7 | 1 | 85.3 |

Table 3: Pharmacokinetics parameters of shortlisted compounds.

| Sr | Compound | Gastrointestinal absorption | BBB permeation | P-glycoprotein substrate | CY-P1A2 inhibitor | CY-P2C19 inhibitor | CY-P2C9 inhibitor | CY-P2D6 inhibitor | CY-P3A4 inhibitor | Skin permeation log Kp ($cm \cdot s^{-1}$) |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 17 | High | No | Yes | No | No | Yes | Yes | Yes | -6.86 |
| 2 | 23 | High | No | Yes | No | No | Yes | Yes | Yes | -6.86 |
| 3 | 24 | High | No | Yes | No | No | Yes | Yes | Yes | -6.86 |
| 4 | 26 | High | Yes | No | No | Yes | Yes | Yes | Yes | -5.63 |
| 5 | 27 | High | Yes | No | No | Yes | Yes | Yes | Yes | -5.63 |
| 6 | 30 | High | Yes | No | No | Yes | Yes | Yes | Yes | -6 |
| 7 | 31 | High | Yes | Yes | No | Yes | Yes | Yes | Yes | -5.98 |
| 8 | 41 | High | Yes | No | No | Yes | Yes | Yes | Yes | -6.1 |
| 9 | 43 | High | Yes | No | No | Yes | Yes | Yes | Yes | -6.1 |
| 10 | 51 | High | No | Yes | No | No | No | No | No | -8.79 |
| 11 | 54 | High | Yes | No | No | No | Yes | Yes | Yes | -6.15 |
| 12 | 56 | High | Yes | No | No | Yes | Yes | Yes | Yes | -6.35 |
| 13 | 57 | High | Yes | No | No | Yes | Yes | Yes | Yes | -6.35 |
| 14 | 59 | High | Yes | Yes | No | Yes | Yes | Yes | Yes | -6.34 |
| 15 | 61 | High | Yes | Yes | No | Yes | Yes | Yes | Yes | -6.73 |
| 16 | 62 | High | No | Yes | No | No | No | Yes | Yes | -8.02 |
| 17 | 63 | High | No | Yes | No | No | No | Yes | Yes | -8.02 |
| 18 | 64 | High | No | Yes | No | No | No | Yes | Yes | -8.02 |

Table 4: Bioavailability and Lipophilicity characteristics of shortlisted compounds

| Sr | Com-pound | Bioavail-ability score | Water solubility (log S) | iLOGP | XLOGP3 | WLOGP | MLOGP | SILICOS-IT log P |
|---|---|---|---|---|---|---|---|---|
| 1 | 17 | 0.55 | Moderately soluble as -4.34 | 3.54 | 2.95 | 2.28 | 2.43 | 2.75 |
| 2 | 23 | 0.55 | Moderately soluble as -4.34 | 3.57 | 2.95 | 2.28 | 2.43 | 2.75 |
| 3 | 24 | 0.55 | Moderately soluble as -4.34 | 3.54 | 2.95 | 2.28 | 2.43 | 2.75 |
| 4 | 26 | 0.55 | Moderately soluble as -5.18 | 3.69 | 4.43 | 3.49 | 3.44 | 4.05 |
| 5 | 27 | 0.55 | Moderately soluble as -5.18 | 3.71 | 4.43 | 3.49 | 3.44 | 4.05 |
| 6 | 30 | 0.55 | Moderately soluble as -4.95 | 3.9 | 4.04 | 3.19 | 2.9 | 3.59 |
| 7 | 31 | 0.55 | Moderately soluble as -4.87 | 3.14 | 3.94 | 2.77 | 2.69 | 2.81 |
| 8 | 41 | 0.55 | Poorly soluble as -6.05 | 3.74 | 4.72 | 3.79 | 3.91 | 4.49 |
| 9 | 43 | 0.55 | Poorly soluble as -6.05 | 4.38 | 4.72 | 3.79 | 3.91 | 4.49 |
| 10 | 51 | 0.55 | Soluble as -3.04 | 2.71 | 0.54 | 3.51 | 2.58 | 1.88 |
| 11 | 54 | 0.55 | Moderately soluble as -4.83 | 3.92 | 3.79 | 3.05 | 2.55 | 3.57 |
| 12 | 56 | 0.55 | Moderately soluble as -4.62 | 3.25 | 3.53 | 2.99 | 2.55 | 3.75 |
| 13 | 57 | 0.55 | Moderately soluble as -4.62 | 3.69 | 3.53 | 2.99 | 2.55 | 3.75 |
| 14 | 59 | 0.55 | Moderately soluble as -4.89 | 3.98 | 3.8 | 2.95 | 2.63 | 3.21 |
| 15 | 61 | 0.55 | Moderately soluble as -4.54 | 4 | 3.25 | 2.95 | 2.63 | 3.21 |
| 16 | 62 | 0.55 | Soluble as -3.32 | 2.78 | 1.32 | 2.88 | 2.83 | 2.99 |
| 17 | 63 | 0.55 | Soluble as -3.32 | 3.65 | 1.32 | 2.88 | 2.83 | 2.99 |
| 18 | 64 | 0.55 | Soluble as -3.32 | 3.43 | 1.32 | 2.88 | 2.83 | 2.99 |

Table 5: Various Filters for drug likeliness

| Sr | Compound | Lipinski rule | Ghose filter | Veber filter | Egan filter | Muegge filter |
|---|---|---|---|---|---|---|
| 1 | 17 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 2 | 23 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 3 | 24 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 4 | 26 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 5 | 27 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 6 | 30 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 7 | 31 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 8 | 41 | Yes; 1 MW>500 | No, 1 MW>480 | Yes | Yes | Yes |
| 9 | 43 | Yes; 1 MW>500 | No, 1 MW>480 | Yes | Yes | Yes |
| 10 | 51 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 11 | 54 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 12 | 56 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 13 | 57 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 14 | 59 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 15 | 61 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 16 | 62 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 17 | 63 | Yes; 0 violation | Yes | Yes | Yes | Yes |
| 18 | 64 | Yes; 0 violation | Yes | Yes | Yes | Yes |

Table 6: Medicinal Chemistry Properties of shortlisted compounds

| Sr | Compound | Lead likeness | PAINS structural alert | Brenk structural alert | Synthetic accessibility score |
|---|---|---|---|---|---|
| 1 | 17 | 1, MW>350 | 0 alert | 1 alert | 5.18 |
| 2 | 23 | 1, MW>350 | 0 alert | 1 alert | 5.21 |
| 3 | 24 | 1, MW>350 | 0 alert | 1 alert | 5.18 |
| 4 | 26 | 2, MW>350, XLOGP3>3.5 | 0 alert | 1 alert | 5.16 |
| 5 | 27 | 2, MW>350, XLOGP3>3.5 | 0 alert | 1 alert | 5.15 |
| 6 | 30 | 2, MW>350, XLOGP3>3.5 | 0 alert | 1 alert | 5.22 |
| 7 | 31 | 2, MW>350, XLOGP3>3.5 | 0 alert | 2 alert | 5.07 |
| 8 | 41 | 2, MW>350, XLOGP3>3.5 | 0 alert | 2 alert | 5.14 |
| 9 | 43 | 2, MW>350, XLOGP3>3.5 | 0 alert | 2 alert | 5.13 |
| 10 | 51 | 1, MW>350 | 0 alert | 2 alert | 5.27 |
| 11 | 54 | 2, MW>350, XLOGP3>3.5 | 0 alert | 1 alert | 5.14 |
| 12 | 56 | 2, MW>350, XLOGP3>3.5 | 0 alert | 2 alert | 5.14 |
| 13 | 57 | 2, MW>350, XLOGP3>3.5 | 0 alert | 2 alert | 5.13 |
| 14 | 59 | 2, MW>350, XLOGP3>3.5 | 0 alert | 1 alert | 5.25 |
| 15 | 61 | 1, MW>350 | 0 alert | 1 alert | 5.22 |
| 16 | 62 | 1, MW>350 | 0 alert | 1 alert | 5.19 |
| 17 | 63 | 1, MW>350 | 0 alert | 1 alert | 5.18 |
| 18 | 64 | 1, MW>350 | 0 alert | 1 alert | 5.15 |

## Discussion

### *ADME Predictions*

Table 1 shows the Canonical SMILES forms of all the shortlisted molecules with their different physicochemical properties. Table 2 indicates pharmacokinetics prediction, rate of gastrointestinal (GI) absorption was obtained higher for all compounds. The blood-brain permeability was observed negative for compounds 17, 23, 24, 51, 62, 63, 64. For skin permeation (log Kp, cm/s), higher negative value was obtained for 51 (-8.79) and 62, 63,64 (-8.02), Followed the lower negative values for 26, 27 (-5.63). P-glycoprotein substrate activity showed positive for compounds 17, 23, 24, 31, 51, 59, 61, 62, 63, 64 and negative for 26, 27, 30, 41, 43, 54, 56, 57. Compound 51 did not show inhibitory activity for cytochrome p450 as CYP1A2, CYP2C19, CYP2C9, CYP3A4, and CYP2D6. All the compounds showed a negative inhibitory activity against cytochrome p450 CYP1A2.

Table 3 specifies Bioavailability prediction shows similar bioavailability scores for all compounds (0.55). The water solubility data collected for soluble compounds viz. 51 (-3.04), and 62, 63, 64 (-3.32). In Lipophilicity prediction other parameters such as iLOGP, XLOGP3, WLOGP, MLOGP and SILCOS-IT were determined. For iLOGP, among all the compounds, Compound 43 showed the highest value of 4.38, while compound 51 showed the lower value of 2.71. Similarly, for XLOGP3 among all the compounds, Compound 41,43 showed the highest value of 4.72, while compound 51 showed the lower value of 0.54. For WLOGP, among all the compounds, compound 41,43 showed the highest value of 3.79, and lower value of 2.28 were seen for compounds 17, 23, 24. For MLOGP, the lower value of 2.43 was seen for compounds 17, 23, 24, whereas higher value of 3.91 for compound 41, 43 was observed. For SILCOS-IT, compound 41, 43 showed the highest value (4.49) and compound 51 showed the lowest value (1.88).

Drug likeness prediction (Table 4), all compounds applicable for Lipinski rule as 0 violation except compound 41 and 43 was showed Lipinski rule as 1 violation, the same was seen for Ghose filter as well.

Table 5 Predicts Medicinal chemistry friendliness, the lead-likeness obtained 1 violation for around half of the shortlisted compounds except for compounds 26, 27, 30, 31, 41, 43, 54, 56, 57, 59, which showed 2 violations. The PAINS structural alert obtained 0 violation for all compounds, whereas for Brenk structural alert all the molecules showed 1 alert except for 31, 41, 43, 51, 56, 57 which have 2 alerts. The synthetic accessibility score ranged from 5.07 to 5.25 of all the molecules.

## Conclusion:

Crinum species used by traditional medicine practioners for various inflammatory conditions. The present study scientifically validates its effectiveness in alleviating pain due to inflammation in among 18 lead compounds investigated for anti-inflammatory property by*In-silico*analysis;the docking score determined in this study can be correlated with biologicalactivities, which would be a new drug candidate for further development after optimizing the results.

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## Conflict of Interest

The authors declare no conflict of interest.

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