Molecular docking data of E3 ubiquitin-protein ligase WWP1 with compounds from a medicinal plant Justicia adhatoda L.

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Abstract

It is known that E3 ubiquitin-protein ligase WWP1 is linked to oral cancer. Therefore, it is of interest to document molecular docking data of E3 ubiquitin-protein ligase WWP1 with compounds ((Stigmasterol, Pyrazinamide, Vasicinone and Ethambutol)) from a medicinal plant *Justicia adhatoda L* for further consideration.

**Key words:** Oral cancer, WWP1, *Justicia adhatoda L*, molecular docking

**Background:**
Oral cancer is one of the most common malignancies [1-5]. It is known that E3 ubiquitin-protein ligase WWP1 is linked to oral cancer [6-12]. Therefore, it is of interest to document molecular docking data of E3 ubiquitin-protein ligase WWP1 with compounds from a medicinal plant *Justicia adhatoda L* for further consideration.

**Materials and Methods:**

**Preparation of the protein structure:**
The protein structure of WWP1 was downloaded from the Protein Data Bank at 2.1 Å resolution (PDB: ID 1ND7) for this analysis.

**Ligand Preparation:**
The compounds from Justicia adhatoda were downloaded from the PubChem database (Table 1) in (.sdf) format and converted to (.pdb) format using the online Smiles.

**Molecular Docking:**
Molecular docking study was completed using AutoDock vina in The Python Prescription (PyRx) 0.8 virtual screening tool [13]. The grid points in the X, Y and Z-axes are set. The grid core was positioned in the pocket core of the binding site. Protein and ligands were translated to pdbqt formats. Default docking algorithms are used using standard docking protocol. Data is then ranked in the order of rising docking energies. The lowest binding energy of each cluster was considered further [14].

**Results and Discussion:**
Oral cancer is one of the most common malignancies [1-5]. It is known that E3 ubiquitin-protein ligase WWP1 is linked to oral cancer [6-12]. Therefore, it is of interest to document molecular docking data of E3 ubiquitin-protein ligase WWP1 with compounds from a medicinal plant *Justicia adhatoda L* for further consideration.

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Table 2: Molecular docking results of best four compounds obtained from PyRx

<table>
<thead>
<tr>
<th>S.No</th>
<th>Compound Name</th>
<th>Binding Energy kcal/mol</th>
<th>Hydrogen Bond Interaction</th>
<th>Distance</th>
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<tbody>
<tr>
<td>1</td>
<td>Stigmasterol_CID_5280794</td>
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<td>MET-865</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>ASN-892</td>
<td>2</td>
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<tr>
<td>2</td>
<td>Pyrazinamide_CID_1046</td>
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<td>LYS-694</td>
<td>2.5</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>ASP-695</td>
<td>2.5</td>
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<td></td>
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<td></td>
<td>SER-698</td>
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<td></td>
<td>THR-889</td>
<td>2.2</td>
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<td>3</td>
<td>Vasicinone_CID_442935</td>
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<td>SER-679</td>
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<td></td>
<td></td>
<td></td>
<td>PHE-765</td>
<td>1.9</td>
</tr>
</tbody>
</table>
Table 1: List of Selected compounds from *Justicia adhatoda*

<table>
<thead>
<tr>
<th>S.No</th>
<th>Compound Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Amrinone</td>
</tr>
<tr>
<td>2</td>
<td>Anisotine</td>
</tr>
<tr>
<td>3</td>
<td>Sulforaphane</td>
</tr>
<tr>
<td>4</td>
<td>Methyl_ether</td>
</tr>
<tr>
<td>5</td>
<td>Pyrazinamide</td>
</tr>
<tr>
<td>6</td>
<td>Squalene</td>
</tr>
<tr>
<td>7</td>
<td>Stigmasterol</td>
</tr>
<tr>
<td>8</td>
<td>Vasicinone</td>
</tr>
<tr>
<td>9</td>
<td>Vasicoline</td>
</tr>
<tr>
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<td>Hexadecanoic acid</td>
</tr>
<tr>
<td>11</td>
<td>Adhatodine</td>
</tr>
<tr>
<td>12</td>
<td>Ethambutol</td>
</tr>
</tbody>
</table>

**Conclusion:**
We document molecular docking data of E3 ubiquitin-protein ligase WWP1 with compounds (Stigmasterol, Pyrazinamide, Vasicinone and Ethambutol) from a medicinal plant *Justicia adhatoda* L for further consideration in the context of oral cancer.

**References:**
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