

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

Jayaraman Selvaraj<sup>1\*</sup>, Umapathy Vidhya Rekha<sup>2</sup>, Shazia Fathima JH<sup>3</sup>, Venkatacalam Sivabalan<sup>4</sup>, Rajagopal Ponnulakshmi<sup>5</sup>, Veeraraghavan Vishnu Priya<sup>1</sup>, Malathi Kullappan<sup>6</sup>, Radhika nalinakumari Sreekandan<sup>7</sup> Surapaneni Krishna Mohan<sup>8</sup>

<sup>1</sup>Department of Biochemistry, Saveetha Dental College and Hospitals, Saveetha Institute of Medical and Technical Sciences, Saveetha University, Chennai - 600 077, India; <sup>2</sup>Department of Public Health Dentistry, Sree Balaji Dental College and Hospital, Pallikaranai, Chennai-600 100, India; <sup>3</sup>Department of Oral and Maxillofacial Pathology, Ragas Dental College and Hospitals, Chennai, India; <sup>4</sup>Department of Biochemistry, KSR Institute of Dental Sciences and Research, Thiruchengodu-637215, India; <sup>5</sup>Central Research Laboratory, Meenakshi Academy of Higher Education and Research (Deemed to be University), Chennai-600 078, India; <sup>6</sup>Department of Research, Panimalar Medical College Hospital & Research Institute, Varadharajapuram, Poonamallee, Chennai - 600 123, India; <sup>7</sup>Department of Clinical Skills & Simulation, Panimalar Medical College Hospital & Research Institute, Varadharajapuram, Poonamallee, Chennai - 600 123, India; <sup>8</sup>Department of Biochemistry and Department of Clinical Skills & Simulation, Department of Research, Panimalar Medical College Hospital & Research Institute, Varadharajapuram, Poonamallee, Chennai - 600 123. \*Corresponding Author: Dr. Jayaraman Selvaraj - E-mail: jselvaendo@gmail.com; \*Corresponding author - Selvaraj Jayaraman

#### Author contacts:

Selvaraj Jayaraman - jselvaendo@gmail.com; Umapathy Vidhya Rekha- drvidhyarekha@gmail.com; Shazia Fathima JH- shaziafathimarizwan@gmail.com Venkatacalam Sivabalan -biosivabalan@gmail.com; Rajagopal Ponnulakshmi-ramgslaks@gmail.com; Veeraraghavan Vishnupriya-drvisnupriyav@gmail.com; Malathi Kullappan-malak.hari@gmail.com; Radhika nalinakumari Sreekandan-niharakrishna21@gmail.com; Surapaneni Krishna Mohan -krishnamohan.surapaneni@gmail.com.

Received December 29, 2020; Revised January 26, 2021; Accepted January 29, 2021, Published January 31, 2021

DOI: 10.6026/97320630017162

#### Declaration on Publication Ethics:

The author's state that they adhere with COPE guidelines on publishing ethics as described elsewhere at <https://publicationethics.org/>. The authors also undertake that they are not associated with any other third party (governmental or non-governmental agencies) linking with any form of unethical issues connecting to this publication. The authors also declare that they are not withholding any information that is misleading to the publisher in regard to this article.

#### Author responsibility:

The authors are responsible for the content of this article. The editorial and the publisher have taken reasonable steps to check the content of the article in accordance to publishing ethics with adequate peer reviews deposited at PUBLONS.

#### Declaration on official E-mail:

The corresponding author declares that official e-mail from their institution is not available for all authors

## 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 ((Stigmasterol, Pyrazinamide, Vasicinone and Ethambutol)) 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 2.1Å 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].

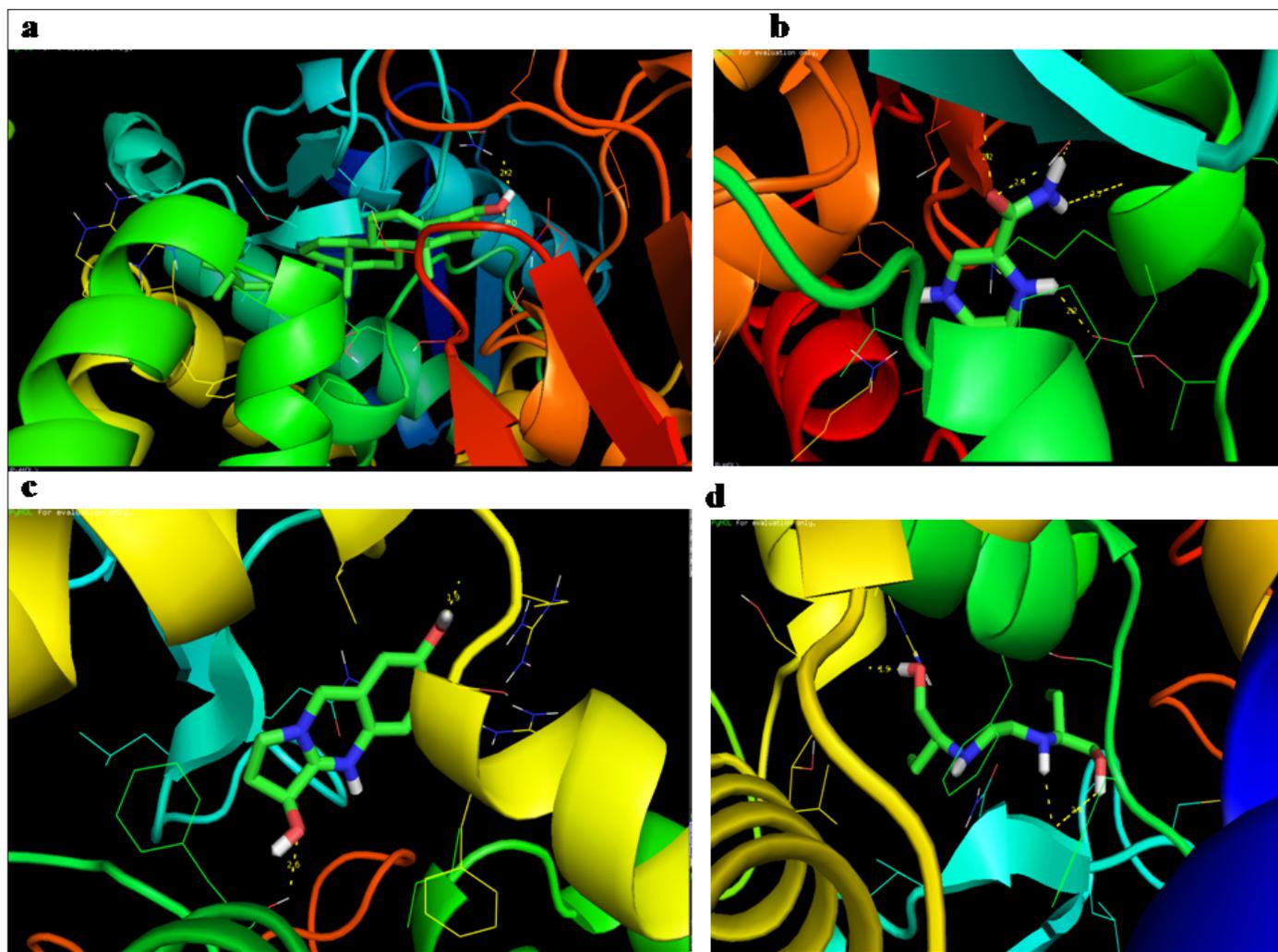
## Results and Discussion:

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. Molecular docking analysis of 12 compounds (Table 1) from *Justicia adhatoda* E3 ubiquitin-protein ligase WWP1 was completed (Table 2). Stigmasterol (-10.21kcal/mol), Pyrazinamide (-8.6 kcal/mol), Vasicinone (-8.2 kcal/mol) and Ethambutol (-7.6 kcal/mol) showed good binding with the WWP1 gene protein target. The interaction of compounds and the target protein was visualized using PyMOL as shown in Figure 1. The amino acids residues MET-865, ASN-892, LYS-694, ASP-695, SER-698, THR-889, SER-679, ARG-767, LEU-641 and PHE-765 were involved in the interaction between the WWP1 and compounds through H-bond formation. Thus, 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.

**Table-2:** Molecular docking results of best four compounds obtained from PyR

S.No	Compound Name	Binding Energy kcal/mol	Hydrogen Bond interaction	Distance
1	Stigmasterol_CID_5280794	-10.1	MET-865 ASN-892	2.2 2
2	Pyrazinamide_CID_1046	-8.6	LYS-694 ASP-695 SER-698	2.5 2.2 2.4
3	Vasicinone_CID_442935	-8.2	THR-889 SER-679 ARG-767	2.2 2.6 1.9
4	Ethambutol_CID_14052	-7.6	LEU-641 PHE-765	2.4 1.9



**Figure 1:** Molecular docking interaction of WWP1 with (a) Stigmasterol; (b) Pyrazinamide; (c) Vasicinone and (d) Ethambutol

**Table 1:** List of Selected compounds from *Justicia adhatoda*

S.No	Compound Name
1	Amrinone
2	Anisotine
3	Sulforaphane
4	Methyl_ether
5	Pyrazinamide
6	Squalene
7	Stigmasterol
8	Vasicinone
9	Vasicoline
10	Hexadecanoic acid

11	Adhatodine
12	Ethambutol

### 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:

- [1] Moore RJ *et al. Ethn Health*. 2001 **6**:165. [PMID: 11696928].
- [2] Petersen PE. *Community Dent Oral Epidemiol*. 2003 **1**:3. [PMID: 15015736].
- [3] Jeng JH *et al. Oral Oncol*. 2001 **37**:477. [PMID: 11435174].
- [4] Diamandis EP *Clin Chim Acta*. 1997 **257**:157. [PMID: 9118561].
- [5] Rak J *et al. Cancer Metastasis Rev*. 2000 **19**:93. [PMID: 11191070].
- [6] Leite KR *et al. Mod Pathol*. 2001 **14**:428. [PMID: 11353053].
- [7] Chen C *et al. Int J Cancer*. 2007 **121**:80. [PMID: 17330240].
- [8] Seo SR *et al. EMBO J*. 2004 **23**:3780. [PMID: 15359284].
- [9] Chen C *et al. Oncogene*. 2007 **26**:2386. [PMID: 17016436].
- [10] Li Y *et al. Cell Death Differ*. 2008 **12**:1941. [PMID: 18806757].
- [11] Lin JH, *et al. Oral Surg Oral Med Oral Pathol Oral Radiol*. 2013 **116**:221. [PMID: 23849376].
- [12] Muhammad SA, *et al. Pharmacogn Mag*. 2015 **11**:S123. [PMID: 26109757].
- [13] Trott O *et al. J Comput Chem*. 2010 **31**:455. [PMID: 19499576].
- [14] Morris GM *et al. J Comput Chem*. 2009 **30**:2785. [PMID: 19399780].
- [15]

Edited by P Kanguane

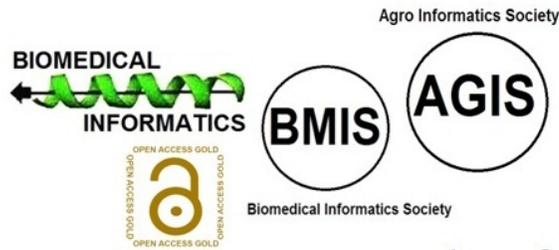
Citation: Selvaraj *et al. Bioinformation* 17(1): 162-166 (2021)

**License statement:** This is an Open Access article which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly credited. This is distributed under the terms of the Creative Commons Attribution License

Articles published in BIOINFORMATION are open for relevant post publication comments and criticisms, which will be published immediately linking to the original article for FREE of cost without open access charges. Comments should be concise, coherent and critical in less than 1000 words.

# BIOINFORMATION

*Discovery at the interface of physical and biological sciences*



since 2005

## BIOINFORMATION

*Discovery at the interface of physical and biological sciences*

*indexed in*

