Institution Logo

Title of the Product/Project

Potential inhibitor of Thymoquinone (CID: 10281) Nigella sativa (Black seed) active compound against COVID 19 in silico study

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PRODUCT ID

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ABSTRACT

SARS-COV-2 was identified in Wuhan city of China in December 2019, a new strain of the coronavirus family. There are no specific drugs available regarding the treatment of the COVID-19. Therefore, in silico screening for natural compounds was required to evaluate their antiviral effect. Molecular docking is the most common type of in-silico study which enables the visualization of binding conformation of ligand to target and produce quantitative in the form of binding energy. Remdesivir is the drug that showed promising results in some COVID-19 patients used as the control in the study. Thymoquinone (CID: 10281) Nigella sativa (Black seed) active compound was used to test its binding affinity towards the main protease and the spike protein using molecular docking. The results from molecular docking indicate that Thymoquinone was able to fit into the binding pocket of the main protease and the spike protein of COVID-19 with highest binding affinity. The analysis obtained from molecular surface supports the postulation above. In conclusion, Thymoquinone showed to be ideal inhibitors compounds for SARS-COV-2. The ligands identified showed a promising result as an effective antiviral for covid-19 and it required further investigation in vitro and in vivo

INTRODUCTION

- Its botanical name is Nigella sativa. It is believed to be indigenous to the Mediterranean region but has been cultivated into other parts of the world including the Arabian peninsula, northern Africa and parts of Asia.
- It is not only a prophetic herb, but it also holds a unique place in the medicine of the Prophet Companies focusing on the fabrication and development of vaccine only.
- They did not find a suitable solution for the management of the infected peoples.
- **COVID 19** responsible for increase in the number of the mortality of the infected patients.
- According to our search there is no agents from natural plants or herbs used or tested as anti COVID-19.

METHODOLOGY

Receptor preparation
- The receptor was retrieved from Protein Data Base (https://www.rcsb.org) .

Ligand preparation
- The ligands were retrieved from PubChem (https://pubchem.ncbi.nlm.nih.gov) in SDF format and by using Pymol software the format was converted to PDB.
- The 3D structure of Thymoquinone (CID: 10281),

Docking procedure
- The molecular docking process was done using PyRx software,
- The receptor and the ligands submitted in PDB format, respectively.
- Vina search space was prepared as the following: Centre (X: -26.2348, Y:14.5426, Z:58.2395) and Dimensions angstrom (X: 46.5578, Y:62.0954, Z: 56.2231)

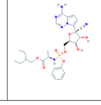
Prediction of ADMET of the ligands
- ADME is known as Adsorption, Distribution, Metabolism and Excretion.
- It's an important component to analyse the pharmacodynamics of the proposed molecules which could be used as therapeutic drugs.
- The online database pkCSM was used to predict ADMET of the ligands by submitting the SMILES strings of the small molecules22.
- The SMILES strings of the ligands obtained from PubChem, submitted into the website and ADMET mode was selected.

PRODUCT DESCRIPTION/ INNOVATION IN BRIEF

- **This invention selected Thymoquinone (CID: 10281) Nigella sativa (Black seed) active compound to be used as promising agent against COVID 19**
- **Tested as antiviral agent against COVID 19 in dry lab.**
- **Showed a potent anti viral effects**
- **Can be considered as an agent for the management of patient infected by this virus**
- **This will be useful in developing new therapies and clinical strategies against the COVID-19 infection.**

METHODOLOGY

Binding Diagram Analysis

Ligand name	Ligand 2D structure	Main protease Binding affinity (kcal/mol)	Spike protein Binding affinity (kcal/mol)
Thymoquinone		5.2	5.6
Remdesivir		7.8	7.8

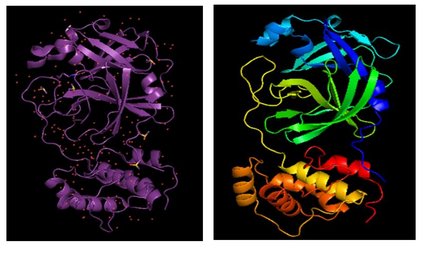


Figure 1. (a) shows the SARS-COV-2 main protease docked with Carmofur; (b) shows Crystal structure of SARA-COV-2 main protease after optimization.

Table 1: Interaction data between the ligand and one control docked with COVID-19 main protease

SHARIAH COMPLIANCES

Black Seed Considered a Universal Remedy The **Prophet Muhammad (Peace be Upon Him)** said in his divine wisdom about the Black seed

"Use this Black seed, it has a cure for every disease except death". (Sahih Bukhari).

SIGNIFICANCES

- Companies focusing on the fabrication and development of vaccine only.
- They did not find a suitable solution for the management of the infected peoples.
- COVID 19 responsible for increase in the number of the mortality of the infected patients.
- There are no specific drugs available in the market and trials regarding the treatment of the COVID-19
- COVID-19 has continued to spread worldwide and causses death of certain percentage of the infected patients

NOVELTY/ ORIGINALITY

- According to our search there is no agents from natural plants or herbs used or tested as anti COVID-19.
- At the present time, there is no approved drug for treating COVID-19 although there have been cases reported as having been treated successfully with compassionate use of remdesivir in the USA.
- Therefore, there is a need to develop new therapeutic drugs to suppress the virus replication.

AWARDS :: PUBLICATION :: PATTERNS

1-Patent Application
2-Paper submitted to Scopus journal under review

Patent Application

Paper under review Scopus