ORIGINAL ARTICLE

# Suplementation of Nigella Sativa as Antioxidant in COVID-19 Patients: *In Silico* Study *via* the Nrf2-Keap1 Pathway

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## ABSTRACT

The human corona virus disease of 2019 is a viral disease that can produce oxidative stress due to reduced antioxidant activity. Black cumin is a plant that can be taken as a supplement to boost antioxidant levels in the body, although the process is still unknown. As a result, the *in silico* method will be used to screen the potential of Nigella Sativa peptide as an antioxidant in this study. Protein tracking was done using the UniProt database (https://www.uniprot.org/), with KEAP1 as the target protein (GDP: 5CGJ). Molecular docking was performed using Patchdock Server and antioxidant activity was determined using https://services.healthtech.dtu.dk/service.php?AnOxPePred-1.0. The researchers concluded that peptides found in Nigella Sativa's NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic protein, had antioxidant potential through suppressing KEAP1 activity with the lowest ACE in Tyr-Tyr-Glu and Cys-Tyr-Tyr.

**Keywords:** COVID-19, KEAP1, Nigella Sativa, Nrf2, Peptide.

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## INTRODUCTION

Human coronavirus disease 2019 (COVID-19) is an infectious disease caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), a single-chain RNA virus that has a capsule, nucleocapsid, spike glycoprotein, and other non-structural proteins.[1,2] There were 4,260,677 confirmed COVID-19 patients in Indonesia between March 2, 2020 and December 20, 2021, with 144,013 deaths.[2]

COVID-19 infection is caused by viruses that enter cells and increase oxygen consumption, causing hypoxia in the cells, which causes oxidative stress and increased activity of antioxidant enzymes like peroxidase, catalase, and superoxide dismutase. Furthermore, oxidative stress can activate a number of transcription factors, including nuclear factor kappa-B (NF κB), p53, HIF-hypoxia-inducible factor 1α, peroxisome proliferator-activated receptor γ (PPAR-γ), β-catenin/Wnt, and Nrf2.[3,4]

The erythroid 2-related nuclear factor protein (Nrf2) is a key protein in the Nrf2/KEAP1 pathway, which controls the antioxidant response. Nrf2 binds to the Kelch ECH Associating Protein 1 (KEAP1) protein when it is inactive. Free Nrf2, on the other hand, will translocate into the nucleus of the cell and trigger the expression of antioxidant genes like superoxide dismutase, catalase, and peroxidase.[3,4]

**Figure 1:** NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic protein sequence of NS

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