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Synthesis, In Silico and Inhibition Evaluations of Carvone Derivatives as Potential Neuraminidase Inhibitors

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Abstract

The pathogenic influenza virus infects the human respiratory tract, causing seasonal outbreaks and pandemics across the globe. Vaccination and anti-influenza drugs are the current strategies used to combat this disease, although new drugs are urgently needed owing to the increasing emergence of antiviral resistance of the existing drugs. Herein, we report the synthesis of a series of carvone derivatives. The compounds were characterized by the FT-IR, ESI-MS, ¹H NMR, and ¹³C NMR spectroscopy, and their binding affinities were evaluated in silico. Molecular docking of the derivatives in the neuraminidase (NA) active site (PDB ID: 3TI6) showed compound 3e to display the best binding energy at −8.35 kcal/mol, comparable with oseltamivir (OTV) (−8.58 kcal/mol), followed by 3b (−8.03 kcal/mol) and 7 (−7.46 kcal/mol). The molecular dynamics simulations of the protein–ligand complexes showed that both 3e-NA and OTV–NA complexes were comparable in stability and

flexibility. Compound 3e also showed the highest inhibition percentage at 1000 mg/mL (60.95%) followed by 3b (59.21%), 7 (54.17%), and 4 (51.14%). Compound 3b gave the highest inhibitory activity of the series with $IC_{50} = 29.53$ mM, followed by 4 (35.50 μ M), 3e (44.13 μ M), and 7 (52.83 μ M). The studies indicate the potential of these derivatives to be designed and developed as effective neuraminidase inhibitors. © Springer Science+Business Media, LLC, part of Springer Nature 2025.

Author keywords

carvone; influenza; molecular docking; molecular dynamics; neuraminidase

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Abstract

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