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

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Source PHARMACEUTICAL CHEMISTRY JOURNAL
DOI: 10.1007/s11094-025-03452-7

Early Access NOV 2025

Indexed 2025-11-15

Document Type Article; Early Access

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 IC50 = 29.53 mM, followed by 4 (35.50 mu M), 3e (44.13 mu M), and 7 (52.83 mu M). The studies indicate the potential of these derivatives to be designed and developed as effective neuraminidase inhibitors.

Keywords

Author Keywords: influenza; neuraminidase; molecular docking; carvone; molecular dynamics

Keywords Plus: ACID-DERIVATIVES; INFLUENZA; DESIGN; LIMONENE; ASSAY

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Categories/ Classification

Research Areas: Pharmacology & Pharmacy

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Chemistry, Medicinal; Pharmacology & Pharmacy

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