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Unveiling mechanism of action of alkaloids from *Macleaya microcarpa* as NF-κB inhibitors for gastric cancer: Insights from network pharmacology, molecular docking, dynamics simulations and ADMET prediction

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Gastric cancer, a highly aggressive malignancy, ranks fifth globally in new cases and deaths in 2022. Natural products from traditional Chinese medicine exhibit potential in cancer therapy. The present study investigates the mechanism of benzophenanthridine alkaloids from *Macleaya microcarpa* as potential anti-gastric cancer agents, targeting the NF-κB-inducing kinase (NIK, protein ID: 4G3F). The results indicate that CPD1 likely modulates the non-canonical NF-κB pathway, with molecular docking revealing a superior binding energy (–9.86 kcal/mol) compared to IMD 0354 (–7.61 kcal/mol). Molecular dynamics simulations over 100 ns confirm stable interactions, with RMSD ranging from 0.20 to 0.25 nm, Rg around 2.1 nm, and SASA from 150 to 165 nm^2, supporting a robust binding profile. *In silico* ADMET analysis demonstrates high intestinal absorption, limited distribution, CYP3A4 metabolism, and a good clearance rate, with no AMES toxicity. These results position CPD1 as a promising NIK inhibitor for gastric cancer therapy.

Keywords: ADMET, Alkaloid, Gastric cancer, *Macleaya microcarpa*, Molecular modeling, Nuclear factor kappa B