

The drug-likeness properties of anti-arthritis curcuma longa compounds curcumin, demethoxy curcumin and bisdemethoxy curcumin: in-silico analysis

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Background and Objectives: Arthritis is a major cause of disability worldwide, with current pharmacological treatments limited by high cost and adverse side effects. Curcuma longa (turmeric) has long been used in traditional medicine, with its curcuminoids—curcumin, demethoxycurcumin (DMC), and bisdemethoxycurcumin (BDMC)—reported to possess anti-inflammatory and antioxidant activities. However, their drug-likeness properties and molecular interactions with arthritis-related biomarkers remain insufficiently characterised. The objectives of this study were to conduct ADMET analysis, to determine the drug-likeness of these compounds and to perform molecular docking of these compounds to see how they interact with the key biomarkers of arthritis. The aim was, to evaluate the drug-likeness properties, protein target predictions, and molecular docking interactions of curcumin, DMC, and BDMC using in silico approaches.

Methods: SwissADME was used to assess pharmacokinetics and drug-likeness, SwissTargetPrediction for protein target prediction, and SwissDock for molecular docking against arthritis biomarkers.

Results: All three curcuminoids complied with Lipinski's rule of five, had favorable bioavailability scores, and showed high gastrointestinal absorption. Curcumin displayed the lowest solubility, while BDMC exhibited superior topological polar surface area, solubility, and blood–brain barrier permeability. Protein target prediction highlighted curcumin's strong binding probabilities to prostaglandin E synthase and inducible nitric oxide synthase. DMC demonstrated moderate interactions, whereas BDMC showed greater association with kinases and G-protein coupled receptors. Docking confirmed stable interactions of all three compounds, with BDMC showing strong binding affinities despite lower predicted probabilities for classical inflammatory enzymes.

Conclusion: Curcuminoids, particularly BDMC, display promising drug-like properties and mechanistic relevance to arthritis management. These findings support their candidacy as complementary anti-arthritic agents, but experimental validation is required to confirm therapeutic potential and safety.