

Investigation of the Anti-Inflammatory Efficacy of Selected Homeopathic Formulation through CFA-Induced Arthritis, Accompanied by an *in silico* Analysis

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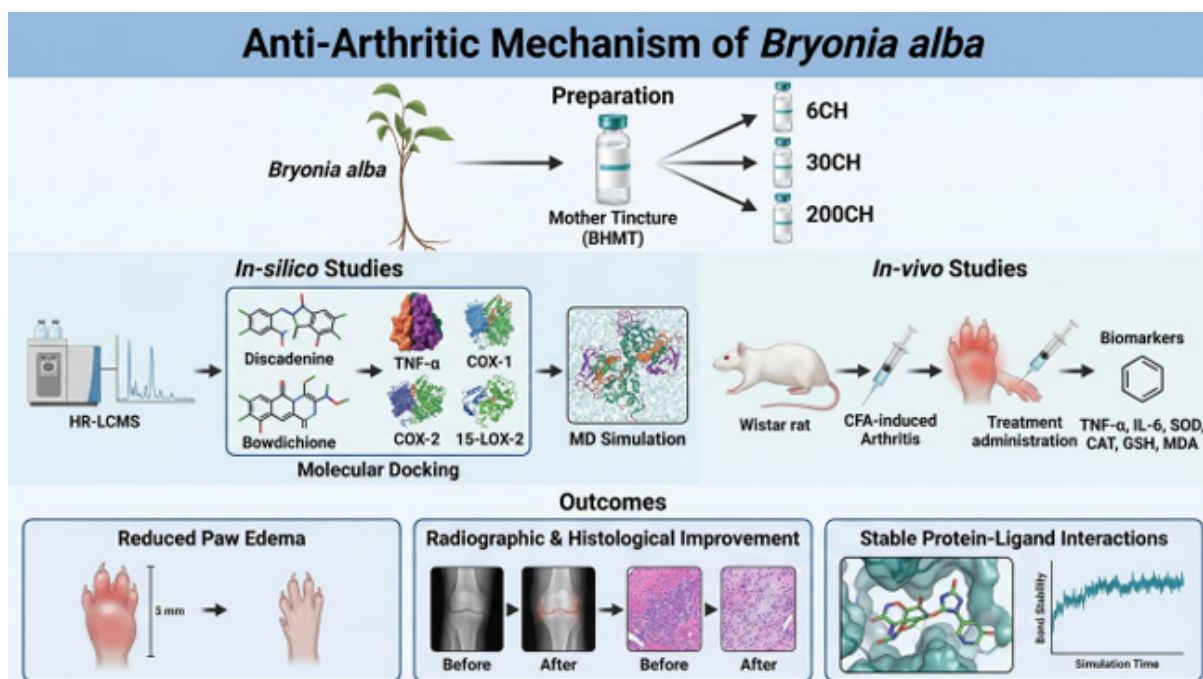
Abstract

Background and Aim: A chronic autoimmune inflammatory disease, rheumatoid arthritis is linked to oxidative stress, increased inflammatory cytokines, and joint damage. The goal of the current study was to assess the anti-arthritic potential of *Bryonia alba* mother tincture (BHMT) and its homeopathic dilutions (6CH, 30CH, and 200CH) utilizing molecular dynamics simulation, HRLCMS profiling, in silico research, ADMET analysis, and in vivo testing in rats with CFA-induced arthritis.

Material and Methods: The phytoconstituents in BHMT and its dilutions were identified by HR-LCMS analysis. Following molecular docking against inflammatory targets such as TNF- α , COX-1, COX-2, and 15-lipoxygenase-2, the identified compounds underwent molecular dynamics modeling and ADMET prediction. In Wistar rats with arthritis induced by Complete Freund's Adjuvant (CFA), anti-arthritic activity was assessed by measuring paw edema, oxidative stress markers (SOD, CAT, GSH, MDA), pro-inflammatory cytokines (TNF- α and IL-6), and radiographic and histological alterations.

Results: Several phytoconstituents in BHMT and their potencies were found by HR-LCMS analysis. With binding scores that were on the same level as or higher than Diclofenac, Discadenine and Bowdichione demonstrated a considerable docking affinity toward inflammatory proteins. While ADMET experiments revealed advantageous pharmacokinetic characteristics, MD modeling verified stable protein-ligand interactions. *Bryonia alba* formulations, especially 30CH and 200CH, were shown to have strong anti-arthritic action in in vivo experiments. This was indicated by decreased paw edema, lowered TNF- α and IL-6 levels, restoration of antioxidant parameters, and improvement in radiographic and histological abnormalities. The results were similar to those of diclofenac treatment.

Conclusion: *Bryonia alba* has significant anti-inflammatory and anti-arthritic potential, according to the study. While in vivo results showed increased biological activity in potentized formulations, particularly 30CH and 200CH, HR-LCMS, docking, and MD modeling confirmed the medicinal importance of phytoconstituents contained in the mother tincture. These results suggest more research into the molecular mechanisms of potentized medications and suggest that further homeopathic potentization studies are required to understand the biological responses.



List of Abbreviations:

ADMET: Absorption, Distribution, Metabolism, Excretion, and Toxicology

CAT: Catalase

COX: Cyclooxygenase

B6CH: *Bryonia Alba* 6 Centesimal Hahnemannian

B30CH: *Bryonia Alba* 30 Centesimal Hahnemannian

B200CH: *Bryonia Alba* 200 Centesimal Hahnemannian

BHMT: *Bryonia Alba* Homeopathic Mother Tincture

GSH: glutathione

HR-LCMS: High-Resolution Liquid Chromatography-Mass Spectrometry

LPO: Lipid peroxidase

NSAIDs: Non-Steroidal Anti-Inflammatory Drugs

SOD: Superoxide dismutase

TNF: Tumor Necrosis Factor

MD simulation: Molecular dynamics

Keywords

Anti-inflammatory, *Bryonia Alba*, Homeopathy, *in-silico*, potency.