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ARTICLE

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DECODING BIOACTIVE COMPOUNDS FROM THE RIVER GANGA BY TARGETING HUMAN CXCR4 FOR ADVANCES IN REGENERATIVE MEDICINE

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The human C-X-C chemokine receptor 4 (CXCR4), indicating its potential as a CXCR4-targeting drug in regenerative therapy, calcium alginate, hyaluronic acid, chitin, and a collagen prolyl hydroxylase inhibitor toward the human CXCR4 receptor. The research employed molecular docking, active site prediction, and molecular dynamics simulations to evaluate how strongly four bioactive compounds interact with the target. Although the other compounds showed diminished binding capacity, they are known to facilitate regeneration through extracellular matrix remodeling and biochemical signaling. The findings highlight the effectiveness of bioinformatics techniques in evaluating natural substances for medicinal purposes and suggest further experimental investigations.