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Research Article

Masoprocol: a promising candidate for targeting insulin resistance by inhibiting resistin with optimal druglikeness Potentials: an *in silico* approach

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Abstract

Resistin is a cysteine-rich secretory hormone that induces resistance to insulin, and its elevated expression is correlated with the onset of diabetes and several related metabolic disorders. Resistin performs its inhibitory role by connecting three identical

subunits through Cys22-based disulfide linkages. The necessity to inhibit the formation of resistin trimer is one of the essential means to prevent the aggravation of diabetes

clinically approved drugs to find the most potent one to inhibit resistin with the best pharmacokinetics and drug-likeness properties. A total of 4654 clinically approved drugs were docked against the Cys22 residue of resistin. The top ten drugs with the highest high-precision (XP) docking scores were selected. Ioversol and masoprocol showed the highest XP docking and Molecular Mechanics-Generalized Born Surface Area (MMGBSA) scores, respectively, with double hydrogen bonding with the targeted Cys22. Molecular dynamics (MD) simulations showed that the masoprocol-resistin complex exhibited lower root mean square deviation (RMSD), radius of gyration, and root mean square fluctuation (RMSF) values than those observed in the ioversol-resistin complex. Both drugs induced drastic conformational changes in resistin monomer interactions. However, ioversol did not prove satisfying drug-likeness properties, while masoprocol showed the most favourable pharmacokinetic and drug-likeness properties. This study has demonstrated that masoprocol offers a novel inhibitory effect on resistin with the highest ligand affinity, making it a promising drug for combating insulin resistance.

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No potential conflict of interest was reported by the author(s).

Authors contribution

MBSA: Conceptualization, Methodology, Writing- Original draft preparation. **SAK, SA,** and **HOH**: Software, Data curation, Writing- Reviewing and Editing: **IMBA** and **DHO**: