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(57) Abstract :
The present invention discloses a biomolecular approach to obesity management by targeting Diacylglycerol acyltransferase (DGAT), the key enzyme involved in triacylglycerol (TG) synthesis. Molecular docking studies were conducted using VlifeMDS to identify potent inhibitors against DGAT1 and DGAT2. Ligands such as triterpenoid betulinic acid, 2-phenyl oxazole, niacin, and N-ethylmaleimide exhibited strong binding affinity, with docking scores ranging from –4.45 to –4.05 kcal/mol—comparable to the enzyme's natural substrate. The active site residues involved in ligand binding were identified for both DGAT isoforms, revealing crucial molecular interactions. The study confirms that these selected ligands can effectively inhibit TG formation, offering a promising strategy for anti-obesity drug development.

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