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# Synthesis, characterization, and molecular docking analysis of triazole, Schiff bases, oxazepane, and oxazepine derivatives against breast cancer targets

**Suha Khudaida Khalaf and Ammar H. Al-Sabawi***
Department of Chemistry, College of Science, University of Mosul, Mosul, Iraq.

**ABSTRACT** This study describes the development of new heterocyclic compounds using a three-step method: Formation of *tris*(4-aminotriazole-3-thione) (**A1**) from nitrilotriacetic acid and thiocarbohydrazide, derivatization to Schiff bases (**A2–A11**) using various aromatic aldehydes, and subsequent conversion to oxazepanes (**A12–A16**) and oxazepines (**A17–A21**) via reaction with phthalic anhydride or succinic anhydride in dry benzene. Molecular docking studies against human epidermal growth factor receptors 2 and phosphoinositide 3-kinase showed strong binding affinities (ΔG values up to −10.2 kcal/mol), indicating promising anticancer potential.

**KEY WORDS:** 4-Aminotriazole-3-thione, Breast cancer, Nitrilotriacetic acid, Oxazepane, Oxazepine, Schiff bases, Thiocarbohydrazide.

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