البحث السابع

رقم البحث فى قائمة الأبحاث الكلية (29)

عنوان البحث باللغة الإنجليزية:

Title:

Novel Imidazoles from Guanylhydrazone: Synthesis, Computational, and Molecular Docking Studies as α-Amylase Inhibitors for Type 2 Diabetes Management

اسم المجلة المنشور بها البحث وسنة النشر

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Abstract:

This study reports a facile synthesis of novel imidazole derivatives as potential α-amylase inhibitors for type 2 diabetes management. Starting with readily available precursors (p-chloroacetophenone and aminoguanidine), guanylhydrazone 3 was synthesized and further functionalized with hydrazonoyl halides or dimethyl acetylenedicarboxylate (DMAD) under mild conditions to yield imidazole derivatives 6a–e and imidazolone 14. Structures were confirmed by IR, NMR, and MS. Tautomeric equilibria (azo vs. hydrazo forms) in compounds 6a–e and 9a–f were resolved via NMR and DFT/B3LYP-D3/6-311G++** calculations, which confirmed the azo tautomers as energetically favored (ΔG = − 2.1 to − 4.8 kcal/mol). Molecular docking against human α-amylase revealed compounds 6c, 6d, 9a, 9b, 9c, and 9d as top candidates, exhibiting strong binding affinities (− 9.2 to − 11.4 kcal/mol) through hydrogen bonding and hydrophobic interactions with the active site. ADMET profiling indicated favorable pharmacokinetic properties, including intestinal absorption and low hepatotoxicity. This work

highlights both a versatile synthetic strategy for imidazole-based scaffolds and their therapeutic potential as antidiabetic agents, meriting further preclinical validation.

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