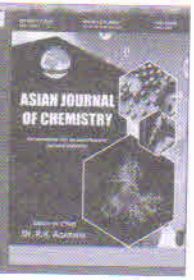
Asian Journal of Chemistry; Vol. 38, No. 2 (2026), 411-416

ASIAN JOURNAL OF CHEMISTRY

https://doi.org/10.14233/ajchem.2026.35020



Synthesis, Characterisation, Molecular Docking and Biological Response of Some New Xylenol Analogues

A. SARAH GRACE[1], L. THANGAVELU[2], M. RUBASRIGAYATHRI[3], T. VIJAYALAKSHMI[3], S.A. SRI HARISH[3], T.A. SHIREEN FARZHANA[4], M. PAVITHRA[4] and S. FULORIA[1,*]

[1]Pharmaceutical Chemistry Unit, Faculty of Pharmacy, AIMST University, Bedong 08100, Kedah, Malaysia
[2]Center for Global Health Research, Saveetha Medical College, Saveetha Institute of Medical and Technical Sciences, Chennai-600077, India
[3]Department of Biochemistry, Saveetha Medical College, Saveetha Institute of Medical and Technical Sciences, Saveetha University, Chennai-600077, India
[4]Department of Microbiology, Saveetha Medical College, Saveetha Institute of Medical and Technical Sciences, Saveetha University, Chennai-600077, India

*Corresponding author: E-mail: shivkanya_fuloria@aimst.edu.my

Received: 7 October 2025 *Accepted*: 5 January 2026 *Published online*: 31 January 2026 AJC-22258

Owing to the versatile biochemical properties of xylenols, the current study was intended to synthesize and characterize some new xylenol analogues (NXAs). The NXAs were evaluated for *in vitro* inhibitory activity against osteomyelitis triggering pathogens (*S. aureus* and *E. coli*), followed by *in silico* AutoDock studies against their key proteins. The NXAs synthesis involved substituted xylenol (**1**) esterification, hydrazination and subsequent treatment with 4-aminoacetophenone to yield intermediate N-(1-(4-aminophenyl)ethylidene)-2-(2,3-dimethylphenoxy)acetohydrazide (**4**), which was further treated with different aromatic aldehydes to yield *N*-(1-(4-((substituted benzylidene)-amino)phenyl)ethylidene)-2-(2,3-dimethylphenoxy)acetohydrazide (**5a-g**) following condensation reaction. The synthesised NXAs were characterised using ATR-IR, ^{1}H NMR, ^{13}C NMR and mass spectrometry. The characterised NXAs were further evaluated for their *in vitro* inhibitory activity against the osteomyelitis-triggering pathogens *S. aureus* and *E. coli*, followed by *in silico* binding affinity studies using AutoDock against their respective key proteins, DNA gyrase B (PDB ID: 4URM) and UDP-N-acetylglucosamine enolpyruvyl transferase (PDB ID: 1UAE). Present investigation concludes synthesis and characterisation success of NXAs and high inhibitory potential against osteomyelitis triggering pathogens and binding affinity with their respective proteins 4URM and 1UAE. Present study recommends that in future the synthesised NXAs of this study should be further subjected to preclinical evaluation for osteomyelitis treatment.

Keywords: Azomethine, Xylenols, Docking studies, Biological activities.