



Synthesis, Antibacterial Activities and Molecular Docking Studies of Ethyl 3-(4-Substituted Phenyl) Propanoates as Targeted Antibiotics

Sivakumar RAMARAJ ^{1*}, Pradeepchandran R. VASANTHAKUMARI ²,
Jayaveera K. NARASIMHA ³, Vijaiand RAJARATHNAM ¹,
Kumarmallasivan PALANI ¹, Arulraj PANNNEERSELVAM ¹ & Venkatnarayanan RAMASAMY ¹

¹ Department of Pharmaceutical Chemistry, RVS College of Pharmaceutical Sciences,
Sulur, Coimbatore- 641 402. Tamilnadu, India.

² Department of Pharmacy, Narayana College of Pharmacy, Nellore, Andrapradesh. India.

³ Jawaharlal Nehru Technological University of college of Engineering,
Anantapur-515 002, Andrapradesh. India.

SUMMARY. Type II fatty acid synthesis (FAS II) pathway has been recently reported as an attractive targeting for their efficacy against infections caused by multi-resistant Gram-positive and Gram-negative bacteria. Among the related FAS II enzymes, beta ketoacyl-acyl carrier protein synthase (KAS), is an essential target for novel antibacterial drug design. Five novel Ethyl-3-(4-substituted phenyl) propanoates have been synthesized, characterized and screened for antibacterial activity. The inhibitory activities against *Escherichia coli* b-ketoacyl-acyl carrier protein synthase III (ecKAS III) were investigated by molecular docking simulation. Compounds which possess both good inhibitory activity and well binding affinities were compared their antibacterial activities against gram negative and gram-positive bacterial strains were tested, expecting to exploit potent antibacterial agent with broad-spectrum antibiotics activity. Compounds 4b, 4c, 4d exhibits significant activity and ethyl-3-(4-chlorophenyl)propanoate (4b) exhibits highest antibacterial activity against all the bacteria among the synthesized compounds.

KEY WORDS: Cinnamic esters, Antibacterial activity, Autodock, ecKAS III.

* Author to whom correspondence should be addressed. *E-mail:* andrilan@rediffmail.com