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RESEARCH ARTICLE

Luminescence, circular dichroism and *in silico* studies of binding interaction of synthesized naphthylchalcone derivatives with bovine serum albumin

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Abstract

Chalcones possess various biological properties, for example, antimicrobial, anti-inflammatory, analgesic, antimalarial, anticancer, antiprotozoal and antitubercular activity. In this study, naphthylchalcone derivatives were synthesized and characterized using ^{1}H NMR ^{13}C NMR, Fourier transform infrared and mass techniques. Yields for all derivatives were found to be >90%. Protein–drug interactions influence the absorption, distribution, metabolism and excretion (ADME) properties of a drug. Therefore, to establish whether the synthesized naphthylchalcone derivatives can be used as drugs, their binding interaction toward a serum protein (bovine serum albumin) was investigated using fluorescence, circular dichroism and molecular docking techniques under physiological conditions. Fluorescence quenching of the protein in the presence of naphthylchalcone derivatives, and other derived parameters such as association constants, number of binding sites and static quenching involving confirmed non-covalent binding interactions in the protein–ligand complex were observed. Circular dichroism clearly showed changes in the secondary structure of the protein in the presence of naphthylchalcones, indicating binding between the derivatives and the serum protein. Molecular modelling further confirmed the binding mode of naphthylchalcone derivatives in bovine serum albumin. A site-specific molecular docking study of naphthylchalcone derivatives with serum albumin showed that binding took place primarily in the aromatic low helix and then in subdomain II. The dominance of hydrophobic, hydrophilic and hydrogen bonding was clearly visible and was responsible for stabilization of the complex.

KEYWORDS

bovine serum albumin, circular dichroism, docking, luminescence, quenching

1 | INTRODUCTION

According to the World Health Organization Tuberculosis Report 2015, in 2014, there were 9.6 million cases of tuberculosis worldwide, 23% of which were in India. Currently, streptomycin, rifampicin and isoniazid are used in the treatment of tuberculosis. However, *Mycobacterium tuberculi* has developed resistance to these drugs over time; therefore, there is an urgent need to search for new potential antitubercular agents.[1]

Chalcones are well-known intermediates in the synthesis of various heterocyclic compounds. The chalcones have been reported to possess various biological properties, such as antimicrobial, anti-inflammatory, analgesic, vasorelaxant, antimalarial, anticancer, antiprotozoal, antioxidant, antihyperglycaemic, inhibition of chemical mediator release (e.g. interleukin-5, leukotriene B4, tyrosinase and aldose reductase), and antitubercular activities.[2]

Abbreviations used: ADME, Absorption, distribution, metabolism and excretion; Arg, Arginine; Asp, Aspartic acid; BSA, Bovine serum albumin; 2D, Two-dimensional; CD, Circular dichroism; Cys, Cysteine; Glu, Glutamic acid; FTIR, Fourier transform infrared; Leu, Leucine; Lys, Lysine; NMR, Nuclear magnetic resonance spectroscopy; Phe, Phenylalanine; Pro, Proline; Trp, Tryptophan; UV, Ultraviolet; Val, Valine; Vis, Visible

