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Molecular Docking Studies of Some Novel Sulfonamides Containing 4-Azidomethyl Coumarin

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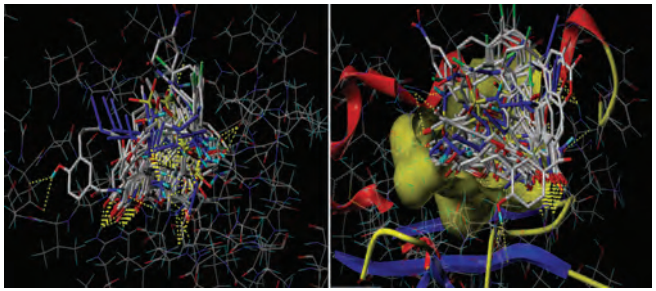
ABSTRACT In this paper, Surflex docking has been carried out on a series (25 sulfonamides containing 4-azidomethyl coumarin derivatives) of *Staphylococcus aureus* inhibitors, using the SYBYL-X 2.0 package (Tripos Inc., St. Louis, USA). Surflex docking studies revealed that the sulfonamide linkage to the coumarins was significant for binding to the receptor, and it is also found that the pattern of binding of tested compounds is same as that of the ligand novobiocin; this, in turn, helped us in understanding the specific activity of compounds.



KEYWORDS Molecular docking, Sulfonamides, 4-azidomethyl coumarin.