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A Docking Study of Relationship between Point Mutations & Ciprofloxacin Resistance in *Campylobacter Jejuni*

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ABSTRACT: Campylobacter bacteria are a major cause of food borne diarrheal illness in developing as well as developed countries. Its incidence rate is higher as compared to the infections caused by S*almonella* species, *Shigella* species, or *Escherichia coli* O157:H7. Fluoroquinolones class of drug is usually employed against campylobacter infections. But antimicrobial resistant *campylobacter* strains have been emerging throughout the world at an alarming rate and irrational use of antibiotics in animals has accelerated it more. *Campylobacter* resistance to fluoroquinolones mainly involves mutation in the gyrA gene encoding for subunit A of DNA Gyrase enzyme. In the present work, docking studies are exploited to understand the ciprofloxacin resistance in *Campylobacter jejuni* at structural level. gyrA structure for *C. jejuni* was modeled using *E. coli* gyrA (1AB4) as template. Two mutants were built with amino acid substitutions at 86 and 104 positions (Thr86Ile and a double mutant Thr86Ile& Pro104Ser) in Discovery Studio. The docking studies against ciprofloxacin (Pubchem Id: 2764) were carried out in LeadIT software, a product of BiosolveIT. It was observed that docking scores were -11.19, -10.91, -10.88 kcal/mol for wild, Thr86Ile, Thr86Ile & Pro104Ser respectively which reproduce the experimental results (0.06, 8, 16 µg/ml MIC values for wild, Thr86Ile, Thr86Ile & Pro104Ser respectively) for ciprofloxacin resistance in C. jejuni isolates in a study carried out by Zirenstein *et* al. Our study allows for the assessment of these point mutations, corresponding to clinically relevant resistance levels to ciprofloxacin.

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