

Minimum free energy pathways of ciprofloxacin and enrofloxacin across OmpC porin of *E. coli*

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The outer membrane of the Gram-negative bacteria, *E. coli* forms a potent physical barrier to antimicrobial agents. The presence of the OmpC porin in outer membrane leads to a potential permeation pathway for the antibiotics to the periplasmic space of the cell [1]. However, there is a significant lack of knowledge regarding the permeation routes taken by different classes of antibiotic molecules thorough this pore. With the help of the metadynamics simulations technique [2,3] and the string method [4] we developed a protocol to characterize the permeation pathway and the rate-limiting molecular interactions underlying the transport of ciprofloxacin and enrofloxacin across the OmpC porin. The procedure has potential to build structure-function relationships between different porins and antibiotic molecules and thereby to aid the development of future antibiotics.

References

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