Carbapenem resistance gene crisis in A. baumannii: A computational analysis

ABSTRACT

Acinetobacter baumannii (A. baumannii) is one of the members of ESKAPE bacteria which is considered multidrug resistant globally. The objective of this study is to determine the protein docking of different ARGs in A. baumannii. In silico analysis of antibiotic resistance genes against carbapenem are the blaOXA-51, blaOXA-23, blaOXA-58, blaOXA-24, blaOXA-143, NMD-1 and IMP-1 in A. baumannii. The doripenem, imipenem and meropenem were docked to blaOXA-51 and blaOXA-23 using PyRx. The top docking energy was − 5.5 Kcal/mol by imipenem and doripenem and meropenem showed a binding score of -5. 2Kcal/mol each and blaOXA-23 energy was − 4.3 Kcal/mol by imipenem and meropenem showed a binding score of -2.3 Kcal/mol, while doripenem showed the binding score of -3.4 Kcal/mol. Similarly, doripenem imipenem and meropenem were docked to blaOXA-58, IMP-1, Rec A and blaOXA-143, with docking energy was − 8.8Kcal/mol by doripenem and meropenem each while imipenem showed a binding score of -4.2Kcal/mol and with IMP-1 demonstrated their binding energies. was − 5.7 Kcal/mol by meropenem and doripenem showed a binding score of -5.3Kcal/mol, while imipenem showed a binding score of -4.5 Kcal/mol. And docking energy was − 4.9Kcal/mol by imipenem and meropenem showed binding energy of -3.6Kcal/mol each while doripenem showed a binding score of -3.9Kcal/mol in RecA and with blaOXA-143 docking energy was − 3.0 Kcal/mol by imipenem and meropenem showed a binding score of -1.9Kcal/mol, while doripenem showed the binding score of -2.5 Kcal/mol respectively. Doripenem, imipenem, and meropenem docking findings with blaOXA-24 confirmed their binding energies. Doripenem had the highest docking energy of -5.5 Kcal/mol, meropenem had a binding score of -4.0 Kcal/mol, and imipenem had a binding score of -3.9 Kcal/mol. PyRx was used to dock the doripenem, imipenem, and meropenem to NMD-1. Docking energies for doripenem were all − 4.0Kcal/mol, whereas meropenem had docking energy of -3.3 Kcal/mol and imipenem was − 1.50Kcal/mol.