

4th African Pharma Congress

June 20-21, 2016 Cape Town, South Africa

Hidden activities of known antibiotics revealed by molecular docking of batumin, mupirocin and bacillaen

Oleg Reva¹, Klochko V V², Zhuravel E V³ and Soldatkina M A³

¹University of Pretoria, South Africa

²Institute of Microbiology and Virology, Ukraine

³R.E.Kavetsky Institute of Experimental Pathology, Ukraine

Antibiotics of the family mupirocin/batumin/bacillaen encoded by larger NRPS-PKS operons are secondary metabolites of many phylogenetically unrelated bacteria from *Pseudomonas* to *Bacillus*. Mupirocin and batumin were found to be active against drug MRSA *Staphylococcus aureus*, but the biological role of these compounds synthesized but several strains of *Pseudomonas* from rhizosphere remained unclear. In this study we used molecular docking approaches and querying of predicted chemical structures through the PharmaDB database of designed pharmacophores to identify possible molecular targets for these antibiotics. The mechanism of inhibition of *S. aureus* by targeting tRNA synthetases by these antibiotics was confirmed. Additionally, it was found that mupirocin, batumin and bacillaen might target bacterial MotB flagellar motor switch protein. Inhibition of the flagellar movement of phytopathogenic bacteria by mupirocin and batumin was proved experimentally. Other predicted possible targets for these antibiotics were several tumor suppressors. Screening of the activity of batumin on the LLC (Lewis lung carcinoma) cell lines showed a promising activity by the mechanism of cell cycle arrest at G1/S checkpoint via activation of retinoblastoma protein and down-regulation of the cyclin D1. This study showed that the known antibiotics may have much wider range of activities. Modern methods of computational analysis and modeling of molecular interactions will help in finding non-traditional areas of application of the old antibiotics instead of designing new ones.

Biography

Oleg Reva has completed his PhD from Kiev State University, Ukraine and Postdoctoral studies from High School of Medicine, Hannover, Germany. He is an Associate Professor in the Centre for Bioinformatics and Computational Biology at the University of Pretoria. He has published more than 90 papers in reputed journals, H-index 20, NRF rating C2.

oleg.reva@up.ac.za

Notes: