Abstract:

Development of resistance against different antibiotics by different pathogens has necessitated the continuous development of new drugs. To continue this process for finding and developing new drugs against resistant pathogens the current study was designed to explore potent inhibitors for the target molecules of *Acinetobacter baumannii*, *Escherichia coli, Methicillin Resistant Staphylococcus aureus (MRSA)* isolated from surgical wound infections. For this purpose, an *in silico* virtual screening of natural and synthetic compounds against specific target molecules was performed. Resultantly, the screened compounds as potent inhibitors present in plant extracts/oils were used to find their antibacterial activity against the aforementioned bacteria isolated from surgical wounds. The extracts/oils of herbs/plants, possessing the screened compounds in larger amounts, were selected for antibacterial activity including; *Thymus vulgaris* (thyme), *Oreganum vulgare* (oregano), *Eucalyptous globulus (Eucalyptous)*, *Elettatia cardamomum (Cardamom oil)*. For *in vitro* analysis the essential oils of these herbs were used. In first step for *in-silico* analysis the selected target enoyl-ACP-reductase, Tyrosine t-RNA Synthetase, Dihydrofolate reductase, DNA gyrase, Pyruvate kinase (with pdb codes 4ZJU,6BQY,5CCC,1AB4,6H5O,3TO5) were screened or docked by using two databases ZINC and Database of natural compounds. Following the three levels of screening procedure including; primary (on the basis of lowest binding energy), secondary (on the basis of higher non-covalent interactions) and tertiary (on the basis of Lipinski rule of five) the final molecules selected from ZINC were with their database IDs as ZINC_00062807, ZINC_03858696, ZINC_04646957, ZINC_08439396, ZINC_04156083 against *A. baumannii* and *MRSA* and those from database of natural compounds were; carvacrol 20 (mol ID 98), alpha-terpene (mol ID 19) and its analogues against *A.baumannii*, carvacrol 20 (mol ID 01), thymol 17 (mol ID 67),thymol 02 (mol ID 06) and its analogues against *E.coli,* and 1,8-cineol (mol ID 06) against *MRSA*, with positive drug score. Therefore, the screened compounds in this study are of importance as drug leads and can be developed as an active drug in near future.