Jose Ignacio Bueso-Bordils et al., Med chem (Los Angeles) 2018, Volume 8
DOI: 10.4172/2161-0444-C1-040

Obtention of minimum inhibitory concentration prediction equations for antibacterial quinolones versus two gram-positive and two gram-negative pathogenic bacteria

Jose Ignacio Bueso-Bordils, Pedro Aleman-Lopez, Antonio Falcó Montesinos, Beatriz Suay-Garcia, Teresa Perez-Gracia, Luis Lahuerta Zamora, Rafael V Martín-Algarra and **Gerardo M Antón-Fos**
CEU Cardenal Herrera University, Spain

The search for new molecules with therapeutic activity is a laborious process with an elevated economic cost. To find a new therapeutic activity for a compound which is provided with pharmacological and toxicological information mean an important saving of money and time which improves its pharmaceutical development as a new drug. Among the different methods used for this purpose, molecular topology has showed to be a useful tool to find quantitative relationships between chemical structure and activity. In this work, a multilinear regression analysis has been carried out in order to look for functions capable of accurately predicting a series of biological properties of a group of quinolones, widely used nowadays because of their broad spectrum activity, well tolerance profile and advantageous pharmacokinetic properties. In order to establish quantitative relationships, it is necessary to numerically describe the chemical structure of compounds by means of topological indices. The studied activities were minimum inhibitory concentration of 50 against *Proteus vulgaris* and *Staphylococcus epidermidis;* and minimum inhibitory concentration of 90 against *Clostridium perfringens* and *Haemophilus influenzae*. The species targeted in this study are very common human pathogens. Intercorrelation, Y-randomization and cross-validation by using leave-one-out test were also performed in order to assess the stability and the prediction ability of the functions selected.

Biography

Jose Ignacio Bueso-Bordils has completed his PhD from CEU Cardenal Herrera University. He is an Associate Professor at CEU Cardenal Herrera University. He has published three papers in reputed international journals, including *European Journal of Medicinal Chemistry*.

jose.bueso@uchceu.es