Abstract

QSAR Analysis of Antibacterial and Antifungal Activity of Novel 2-Morpholinoquinoline Analogs [†]

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The present study is focused on the chemometric QSAR analysis of antifungal and antibacterial activity of novel 2-morpholinoquinoline analogs and their molecular structure described by in silico molecular descriptors. The results of antifungal activity have taken into account *Aspergillus fumigatus* (MTCC 3008) and *Candida albicans* (MTCC 227), while antibacterial activity included Gram positive bacteria (*Clostridium tetani* MTCC 449, *Streptococcus pneumonia* MTCC 1936 and *Bacillus subtilis* MTCC441) and Gram negative bacteria (*Vibrio cholerae* MTCC 3906, *Salmonella typhi* MTCC 98 and *Escherichia coli* MTCC 443). The experimental results of the antimicrobial analysis of studied compounds have been taken from the literature [1]. In the QSAR modeling the chloramphenicol, ciprofloxacin, ampicillin and norfloxacin were used as the standard antibacterial therapeutics. The QSAR modeling has been carried out on the basis of the in silico molecular descriptors (physico-chemical, lipophilicity, topological and absorption, distribution, metabolism, excretion and toxicity—ADMET descriptors) applying linear and multiple linear regression methods, as well as a cross-validation approach. The obtained high-quality models can be considered useful in prediction of the antifungal and antibacterial activity of not yet synthesized structurally similar compounds as well as a contribution to the development of new antimicrobial agents. The studied compounds have been ranked by the sum of ranking differences (SRD) method on the basis of the reference ranking, which was based on the strongest antibacterial and antifungal activities in order to see which compounds express the most potent antimicrobial activity.

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