Identification of adsorptive interactions between cationic pharmaceuticals and Escherichia coli by using linear free energy relationship model

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Estimation of adsorptive interactions between bacterial and pharmaceutical pollutants is necessary to understand environmental fates of the same types of chemical and to develop bacterial-based biosorbent. In present study, we chose Escherichia coli as a model bacteria and determined affinity values for target drugs by adsorption experiments at the low concentrations with pH 6.5. For understanding adsorptive mechanisms, we developed a model by using linear free energy relationship descriptors i.e. excess molar refraction (E), dipolarity/polarizability (S), H-bonding acidity (A), H-bonding basicity (B), McGowan volume (V) and charge interaction of cation (J+). By selecting appropriate LFER descriptors, a prediction model comprised of E, S, A, V and J+ was established; its accuracy is R2=0.941 and standard error=0.157. From the model, we observed that the affinity value was increased as descriptors V, J+ and A increase, while an increase of E and S leads the opposite trend. Here, V is the most important factor and others i.e. E, S, A, and J+ are slightly and similarly contributing to the adsorptive interaction model. These results will be useful to understand the interaction between pharmaceuticals and E. coli.