Quantitative Structure-Activity-Relationship of Para-Substituted Phenol Derivatives to Relate Side-Chain Variation to Antibacterial Activities

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A recent study has been carried out to determine the antimicrobial profile of para-substituted phenols. Modifications to the phenol included the addition of alkyl chains of varying lengths, halogenation, and addition of groups containing heteroatoms. A quantitative structure-activity-relationship (QSAR) analysis was performed using the experimental activities of the molecules. The efficiency of each antimicrobial system was correlated to the molecule's side chain structure. The molecules' properties, such as MOPAC charges and other values associated with the overall size and composition of the side-chains, were calculated and analyzed using SYBYL 7.0 on an HP1230. The objective of the QSAR analysis was to formulate a mathematical model to predict the antibacterial activity of para-substituted phenols using computed properties. This project was supported in part by NSF grant CHE-0116435.