Structurally Modified Celecoxib Analogues for Selective COX-2 Inhibition: a Classical Hansch QSAR Approach

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SUMMARY. **Classical Hansch type quantitative structure-activity relationship (QSAR) has been performed on a set of structurally modified celecoxib analogues for their inhibitory potency and selectivity towards cyclooxygenase isozymes using classical physicochemical and structural parameters. Statistically significant regression models were developed for cyclooxygenase-1 (COX-1), cyclooxygenase-2 (COX-2) inhibitory potency as well as selectivity index. The results of our QSAR study suggest the importance of the molecular size, shape and electronic character of the aromatic ring substituents. Further our investigation provides important structural and physicochemical features for designing potent and selective COX-2 inhibitors within the congener series of compounds.**

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