Quantum?chemical study of the relation between electronic structure and pA2 in a series of 5?substituted tryptamines

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We have analyzed the dependence of the serotonin receptor binding affinity on the electronic and steric reactivity indexes for a group of 5?substituted tryptamines. The approaches employed are a new nonempirical Quantitative Structure?Activity relationship approach and multiple regression analyses. The results suggest that the variation of the receptor binding affinity in 5?substituted tryptamines is related to the variation of the net charge of two atoms and to the steric bulk of the N?substituent. A receptor model is proposed.