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Investigating the Links Between Traditional QSAR. Approach and Molecular Simulations of Protein-Ligand binding

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Simulations for receptor– ligand complexes were carried out for the papain hydrolysis of a series of *N*–benzoylglicine esters in order to look for analogy between traditional QSAR and 3D structural simulations. An aim was to reinterpret traditional QSAR descriptors in light of detailed structural information. Molecular dynamics of 1.5ns length and full structure Local SCF semiempirical (AM1) quantum mechanics calculations were performed. A correlation of $r^2 = 0.697$ was obtained using two kinds of descriptor; atomic charges and watershells, i.e. number of water molecules around certain atoms of ligands. The results emphasize that it is possible replace the electronic descriptors, such as F or σ with accurate atomic charges of complexed molecules in structure–activity relationship studies.