A theoretical study of the inhibition of human 4-hydroxyphenylpyruvate dioxygenase by a series of pyrazalone-quinazolone hybrids

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A Density Functional Theory study was carried out to find relationships between the electronic/molecular structure of a group of pyrazalone-quinazolone hybrids and their inhibition of human 4-hydroxyphenylpyruvate dioxygenase (HPPD). The geometries were fully optimized at the B3LYP/6-31G(d,p) level. A statistically significant equation was obtained. The equivalent 2D pharmacophore was built and some atom-site interactions were suggested. The analysis of the equation and the pharmacophore should provide new information about possible substitution sites for an enhancing of the inhibitory activity.