A theoretical analysis of the inhibition of the VEGFR-2 vascular endothelial growth factor and the anti-proliferative activity against the HepG2 hepatocellular carcinoma cell line by a series of 1-(4-((2-oxoindolin-3-ylidene)amino)phenyl)-3-arylureas

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An analysis of the relationships between electronic structure and the inhibition of the kinase activity of VEGFR-2 was carried out for a series of 1-(4-((2-oxoindolin-3-ylidene)amino)phenyl)-3-arylureas. A similar study was done for the case of cytotoxicity against the HepG2 liver cancer cell line. The Klopman-Peradejordi-Gómez formal method was used. The local atomic reactivity indices were obtained at the B3LYP/6-31G(d, p) level after full geometry optimization. Statistically significant equations relating several local atomic reactivity indices with both activities were obtained. From the results, the corresponding partial 2D pharmacophores were built, containing several sites that can be used for substitution for enhancing affinity.