International Journal of PharmTech Research
CODEN (USA): IJPRIF, ISSN: 0974-4304, ISSN(Online): 2455-9563
Vol.9, No.5, pp 306-314, 2016

QSAR and docking study of p-hydroxyphenylbenzohydrazide derivatives as ACE inhibiters- an antihypertensive agents

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Abstract: In the studies it was found that *p*-hydroxyphenylbenzohydrazide moiety has good biological activity in the form of antihypertensive agents. Therefore derivatives were selected for development of more active human ACE (angiotensin-I-converting enzyme) inhibiters. For QSAR study the substituted- thioxo- thiadiazol- *p*-hydroxyphenylbenzohydrazide derivatives were selected along with biological data to generate 3D-QSAR models. The molecular docking study was done by Glide-Schrodinger software into the angiotensin-I-converting enzyme with PDB code (2xy9). Compounds (4.a-4.n) were considered for docking study. The G-score of the standard ligand i.e. valsartan, in case of docking with 2xy9, was found as -6.11.The G-score of the compounds, (4.d), (4.i), (4.j) and (4.l) were also found as -5.98, -5.70, -5.87 and -5.70 for respectively. The number of H-bond interactions in the standard compound (valsartan) was compared with those of the designed compds. This has indicated the requirement of H-bond interaction for good antihypertensive activity.
Key words: angiotensin-I-converting enzyme**,** QSAR**,** docking, *p*-hydroxyphenylbenzohydrazide, valsartan.

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