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Molecular docking, synthesis and anticonvulsant activity study of some novel hydrazone derivatives

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Series of 4-(4-Ethyl-phenyl)-4-oxo-butyric acid (1-substituted phenyl)-hydrazide and 2-[5-(substituted-phenyl)-5-methyl-4,5-dihydro-[1,3,4]oxadiazole-2-yl)-1-(4-ethyl-phenyl)-ethanone have been synthesized and characterized by NMR, IR, Mass and C, H, N analysis. The docking studies of novel substituted hydrazones and 1,3,4-oxadiazole derivatives have been performed with the AutoDock Vina PyRx-Python Prescription 0.8 in to the 3D structure of the catalytic site of human gamma-aminobutyric acid receptor (PDB ID: 4COF). Best compounds selected on the basis of least binding energies for receptor 4COF among all compounds, H-9, 10, 22, 26 shows least mean binding energy -7.4, -7.0, -7.4 and -7.2 respectively. All these four compounds were evaluated for anticonvulsant activity using maximum electroshock seizures (MES) in male Wister rats (180-220 g). Compounds H-9 shows significant anticonvulsant activity.

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