
**Abstract:** In an endeavor to pursue new strategies beyond conventional ones, energetically optimized, structure based pharmacophore was used for *in silico* anticonvulsant screening in present investigation. The study combines pharmacophore perception with protein-ligand interactions (docking) computed by *BioPredicta* and *MolSign* of VLIFE Molecular Design Suite 4.3.0. We derived energy-optimized pharmacophoric features for six anticonvulsants relevant to (E)-(±) 3-menthone derivatives (J6, J14, J25, J30, J32, J33) to access novel and potent GABA-AT inhibitors. Docking produced the most cases (5/6) with score greater then Vigabatrin, a well known GABA-AT inhibitor with proven clinical anticonvulsant efficacy. The docking results suggest the probable mechanism of anticonvulsant action that leverages the strong H-bonding (LYS329ARG192A) and π-stacking interactions (PHE189A) with GABA-AT receptor.

**Key words:** Pharmacophore, Anticonvulsant, Menthone, GABA-AT, Docking.

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