Article Type: Research Article *Received:* December 11, 2013

Jain J, Bansal SK, Chowdhury P, Sinha R, Tripathi U, Malhotra M. *In silico* pharmacophore validation of anticonvulsant activity of (*E*) (±)-3-menthone derivatives. *Bull. Pharm. Res.* 2013;3(3):146-56.

Abstract: In an endeavor to pursuit 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 (J_6, J_{14}, J_{25}, J_{30}, J_{32}, J_{33}) 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.

References: 22 **Total Pages:** 11 **Cited by:** 00

*Author to whom correspondence should be addressed:
Dr. Jainendra Jain (*jainendrem@gmail.com*)
Department of Pharmaceutical Chemistry, RamEesh Institute of Vocational and Technical Education, Greater Noida, Uttar Pradesh, India