**Article Type:** Research Article *Received:* June 01, 2011

Sharma V, Wakode SR, Lather V, Mathur R, Fernandes MX. Structure based rational drug design of selective phosphodiesterase-4 ligands as anti-inflammatory molecules. *Bull. Pharm. Res.* 2011; 1(2):33-40.

**Abstract:** Phosphodiesterase-4 enzyme (PDE4) has been gaining increasing attention for the last two decades as a pharmacotherapeutic target, as it is involved in the etiology of a variety of pathologies that comprise a majority of inflammation problems concerning respiratory pathway in major aspect. Intense efforts have been directed towards the development of effective and selective PDE4b inhibitors, but not much success has been reported till yet. This is because of the structural similarity between the two isoforms of PDE4, PDE4b (therapeutic effect) and PDE4d (side effect of emesis). Analogues of 1,2-dihydroxy-xanthen-9*H*-one were designed as selective ligands for PDE4b using the structure based drug design. The selectivity was determined by docking of xanthone analogues in PDE4b and PDE4d active sites respectively using GLIDE docking programme from Schrodinger Inc. ADME properties of the designed ligands were also predicted using QikProp from Schrodinger Inc. Interpretation of protein-ligand interactions and binding modes of xanthone analogues showed that these ligands are more selective for PDE4b than for PDE4d.

**Key words:** PDE-4-phosphodiesterase-4, Drug design, Molecular docking, ADME prediction.

**References:** 12 **Total Pages:** 08 **Cited by:** 01

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