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Computer-Aided Design of Negative Allosteric Modulators of Metabotropic Glutamate Receptor 5 (mGluR5): Comparative Molecular Field Analysis of Aryl Ether Derivatives

Chelliah Selvam^{a,*}, Ramasamy Thilagavathi^{b,*}, Balasubramanian Narasimhan^c, Pradeep Kumar^d, Brian C Jordan^a, and Kasturi Ranganna^a

^aDepartment of Pharmaceutical Sciences, College of Pharmacy and Health Sciences, Texas Southern University, Houston, TX 77004, USA

^bDepartment of Biotechnology, Faculty of Engineering, Karpagam Academy of Higher Education, Coimbatore, India

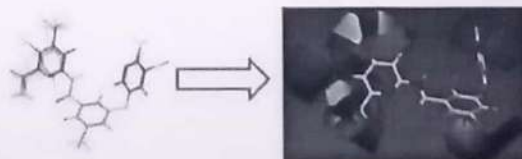
^cDepartment of Pharmaceutical Sciences, Maharshi Dayanand University Rohtak, India

^dCentre for Pharmaceutical Sciences and Natural Products, School of Basic and Applied Sciences, Central University of Punjab, Bathinda, India

Abstract

The metabotropic glutamate receptors (mGlu receptors) have emerged as attractive targets for number of neurological and psychiatric disorders. Recently, mGluR5 negative allosteric modulators (NAMs) have gained considerable attention in pharmacological research. Comparative Molecular Field Analysis (CoMFA) was performed on 73 analogues of aryl ether which were reported as mGluR5 NAMs. The study produced a statistically significant model with high correlation coefficient and good predictive abilities.

Graphical abstract



Keywords

mGluR5; Negative Allosteric Modulators; Aryl ethers; CoMFA; 3-D QSAR

*Corresponding author. Tel.: +1-713-313-7552; chelliahs@tsu.edu. *Corresponding author. Tel.: +91-960-051-3306; thilagavathi@yahoo.com.

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