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Applications of Parallel Synthetic Lead Hopping and Pharmacophore-Based Virtual Screening in the Discovery of Efficient Glycine Receptor Potentiators

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Abstract

Glycine receptors (GlyRs) are pentameric glycine-gated chloride ion channels that are enriched in the brainstem and spinal cord where they have been demonstrated to play a role in central nervous system (CNS) inhibition. Herein we describe two novel classes of glycine receptor potentiators that have been developed using similarity- and property-guided scaffold hopping enabled by parallel synthesis, and pharmacophore-based virtual screening strategies. This effort resulted in the identification of novel, efficient and modular leads having favorable in vitro Download English Version:

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