

Pharmacophore identification and lead optimization for novel antifungals

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Customer Type

Leading Pharmaceutical Company

Software modules

QSAR

LeadGrow

Engine

Background:

Natural products play an important role in drug discovery and have been used for the treatment of various diseases for decades. They constitute a leading source of novel molecules for the development of new drug candidates to treat life threatening infections and other human disorders. To identify such potential drug candidates from nature, different methods have been developed and routinely used in natural product discovery laboratories.

Design Challenge:

Customer has shared a proprietary anti-aspergillus compound obtained from vegetative origin under NDA. The objective of the present study was to develop NCEs with at least anti-aspergillus activity using given natural product.

Retro-synthetic fragmentation approach has been followed to simplify the given tetra cyclic natural product structure. These fragments were searched for similarity with known anti-fungals to get class of anti-fungal compounds with their anti-candida as well as anti-aspergillus activities. A ligand based drug design approach was then utilized to develop new potential anti-fungal candidates.

Application

NCE Design

Techniques

QSAR Analysis

Combinatorial Library

Virtual Screening



