

Title (en)  
COMPUTATIONAL METHOD FOR DESIGNING CHEMICAL STRUCTURES HAVING COMMON FUNCTIONAL CHARACTERISTICS

Title (de)  
RECHENVERFAHREN ZUM ENTWURF VON CHEMISCHEN STRUKTUREN MIT GEMEINSAMEN FUNKTIONELLEN CHARAKTERISTIKEN

Title (fr)  
PROCEDE INFORMATIQUE DE CONCEPTION DE STRUCTURES CHIMIQUES AYANT EN COMMUN DES CARACTERISTIQUES FONCTIONNELLES

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Application  
**EP 96905638 A 19960322**

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Abstract (en)  
[origin: WO9736252A1] The present invention relates to computational methods for designing chemical structures sharing common useful, functional properties based on specific combinations of steric configuration and binding affinity. More particularly the present invention provides a method for producing computer-simulated receptors which functionally mimic biological receptors. The simulated receptors are designed to exhibit optimized selective affinity for known target molecules. Chemical structures are then generated and evolved to exhibit selective affinity for the simulated receptors.

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