

CCG



Scaffold Replacement and Fragment Based Drug Design

The course will focus on fragment-based drug design tools. Combinatorial fragment design and scaffold replacement in the receptor active site will be covered in detail, along with approaches for fragment linking and growing. A method for generating a series of closely related derivatives through medicinal chemistry transformations and the reaction based combinatorial builder will be presented. The use of pharmacophores and 2D/3D descriptors to guide drug design processes will also be discussed.