MedChem & CADD-2013
2nd International Conference on
Medicinal Chemistry & Computer Aided Drug Designing
October 15-17, 2013 Las Vegas, USA

Synthesis of privileged structure libraries for biological evaluation

John Spencer
University of Sussex, UK

Abstract

The synthesis of a diverse drug-like library containing a number of heterocyclic scaffolds is described. Elaborated oxazoles, pyridines, pyrimidines, benzodiazepines, benzotriazepines and biphenyls have been synthesized using a combination of microwave-assisted organic synthesis (MAOS), supported reagents and automatic chromatography. These have been screened against a number of biological targets. Focused libraries have been designed against a number of cancer-relevant targets, namely urokinase, histone deacetylases (HDACs) and p53. Rationalization of these hits has been achieved via molecular modeling and X-ray cocrystallisation studies.

Biography

John Spencer holds a PhD from Strasbourg University and carried out postdoctoral research at the ETH, Zurich. He is a Reader at Sussex, with ten years' industrial leadership in medicinal chemistry (e.g. running parallel synthesis at the James Black Foundation). He is an author of over 80 publications and inventor on 10 patents. His interests are in parallel synthesis, microwave chemistry, catalysis, boron chemistry and fragment based drug discovery.