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Current SAR on HIV: The flow from phenotypic assays via medicinal chemistry to *in silico* design

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Cellular phenotypic assays provide a powerful method to investigate the capability of small molecules to perturb important biological processes. A small library of dihydropyrimidinone (DHPM) derivatives prepared using continuous flow chemistry was tested in phenotypic assays and provided a hit that inhibited the replication of the human immunodeficiency virus (HIV) in cells. Investigation of the structure activity relationships (SAR) around this compound using flow synthesis methodology to rapidly and efficiently generate analogues led to the identification of potent HIV replication inhibitors with promising drug-like properties. Importantly, some of the lead structures inhibit the replication of a drug resistant strain of HIV. Mechanistic studies coupled with 3D *in silico* modeling suggest that these compounds exert their effects by inhibiting the viral RT enzyme.

Biography

Peter Teriete completed his DPhil in biophysics from the University of Oxford, UK and completed postdoctoral studies at the Sanford-Burnham Institute for Medical Research, La Jolla, CA. As a project manager there, he utilizes his extensive expertise in structural biochemistry and biophysical characterization in the design and development of novel small molecule inhibitors of HIV as well as many other pathologies.

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