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Computer-aided design, efficient synthesis and mechanistic studies of serine protease covalent inhibitors

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Covalent serine peptidase inhibitors, Prolyl oligopeptidase, DPP-IV and fibroblast activation protein α are serine exo- and endopeptidases from the S9 family which are targets for cancer, Alzheimer's disease and diabetes type II therapeutics. These 3 enzymes have been inhibited using covalent inhibitors. Our approach combined software development (covalent docking), synthesis, biochemistry and biophysical approaches to develop novel active inhibitors and develop methods for mechanistic studies of covalent inhibition. This integrated approach led to the discovery of a number of novel potent chemical series, novel synthetic methodologies and a better understanding of the covalent inhibition.

Biography

Nicolas Moitessier is an Associate Professor at McGill University, Montréal, Canada. He received his undergraduate training and his PhD from Université Henri Poincaré-Nancy I (France) under the guidance of Dr. Yves Chapleur within the Groupe SUCRES. He carried out thesis research on computer-aided design and synthesis of carbohydrate-based biologically relevant molecules. He was first involved in the design and preparation of IP3 and Adenophostin A mimics using Sharpless asymmetric dihydroxylation as a key reaction. In collaboration with a theoretical chemistry group (headed by Dr. Maigret), he then focused on the computer-aided design and synthesis of carbohydrate-based antagonists of integrins.

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