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Forecaster: A computational tool for drug design and discovery developed by experimentalists for experimentalists

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Abstract

Over the last ten years we have been developing software for drug design and discovery. In order to make them available to experimentalists, efforts were made to automate the processes, thus reducing errors and the need for extensive training. Thus each individual piece of software, including Fitted, a docking program which considers displaceable water molecules, protein flexibility and covalent binding, Impacts, a program for prediction of sites of metabolism of drugs and React, a tool for virtual combinatorial chemistry have been integrated into a web-based platform Forecaster. This platform has then been applied to real case studies. We will present the development of this computational package as well as existing experimental applications and validation. Among these applications are the computer-aided design and synthesis of prolyl oligopeptidase inhibitors that demonstrated high inhibitory potency in cell-based assays and the experimental determination of their major metabolites initially predicted by Impacts.

Biography

Moitessier received his PhD from Université Henri Poincaré (Nancy, France). In 1998, he moved to Montréal where he joined Prof. Hanessian group for post doctoral work. In 2001, he moved back to Nancy to start an academic career then back to Montréal in 2003 (McGill University). His current research interests integrate software development, computational chemistry and organic/medicinal chemistry. He has published over 55 papers and has founded Molecular Forecaster in 2010. In 2008, he received the first Reginald Fessenden Professorship in innovation for the development of the Forecaster drug discovery platform. In 2009, he was awarded the AstraZeneca Award in Chemistry