

The Novartis Kinase Compendium

Overview and Applications

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Kinases are enzymes that catalyze protein phosphorylation, a basic mechanism of regulation of cellular processes. They are key players in signal transduction, cell cycle control and apoptosis. The human kinome is known and contains around 520 members (1.7% of all human genes). The biological function of a substantial number of protein kinases has been identified providing a wealth of therapeutic targets. The structural determinants of protein kinase inhibition (co-factor ATP site directed inhibitors) are well understood making structure-based design a very powerful approach in the optimization or discovery of kinase inhibitors.

Here we present the Novartis Kinase Compendium which is a compilation of the large amount of biological and chemical data available on kinases within Novartis. Our goal is to develop an easily accessible lookup of in-house kinase information linked to the structural information of the X-ray crystal kinase structures available and more particularly the binding mode of the co-crystallized ligand. Due to ATP binding site homology/similarity among all kinases, this Kinase Compendium allow the transference of learning/knowledge across different kinases, deduction of inhibitors for new kinase targets and selectivity profiling of new ligands.