Kinase Library

Designed for discovery of new potent kinase inhibitors

67,385 compounds

Protein kinase inhibitors (PKI) represent an important and still emerging class of targeted therapeutic agents. It is difficult to overestimate the role of protein kinase inhibitors in modern anticancer and immune-oncology therapy. About 40 diverse kinase inhibitors have received FDA approval for the treatment of different cancers, and about 150 kinase-targeted drugs are in clinical phase trials.

In order, to bring ***New Chemistry*** into this well-explored drug discovery field we have carefully designed our Kinase targeted Library, comprising 67,385 compounds. The library is available for cherry picking, as well as for prompt delivery in a **ready-made** format. Pre-plated version of our Kinase Library consists of 64,000 compounds and can be also made in any customized ready-to-screen formats. You can receive multiple benefits in the hit follow-up stages and lead discovery by using our Kinase Library:

- **Hit resupply and hit expansion from dry stock of over 2.6 M compounds.**
- **Straightforward and low-cost analogs synthesis through our REAL Database technology.**
- **Fully customized hit-to-lead project support provided in a timely manner with broad capabilities available on-site.**

You have also an option to screen the librray directly at Enamine. We will be happy to offer you discount on library cost depending on the collaboration scope.

Most popular library formats available for immediate supply

Item	Catalog No.	No of compounds	No of plates	Amount	Plates and format
1	**KNS-64-Y-0**	64 000	200	Any suitable for 1 assay	384-well plates, 320 cpds per plate, first two and last two columns empty
2	**KNS -64-Y-10**	64 000	200	10 µL of 10mM DMSO stock solutions	384-well plates, 320 cpds per plate, first two and last two columns empty
3	**KNS -64-Y-50**	64 000	200	50 µL of 10mM DMSO solutions	384-well plates, 320 cpds per plate, first two and last two columns empty

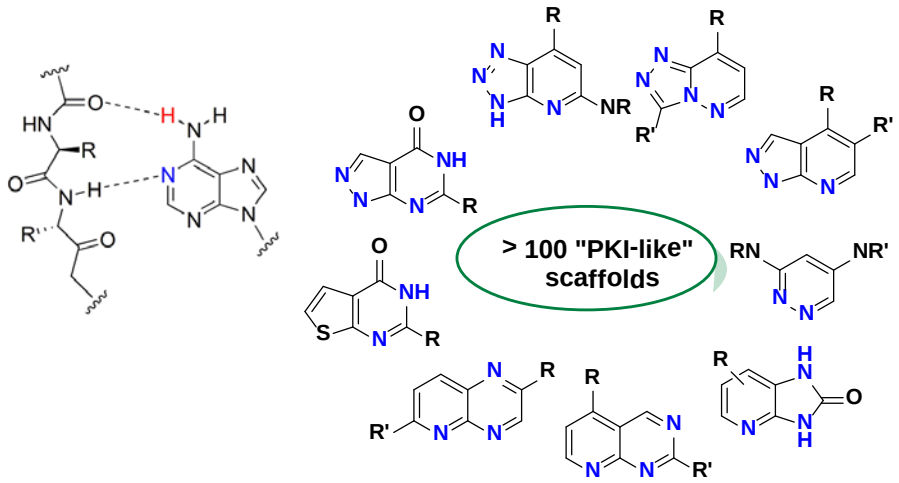
Library Design

In spite of extensive studies and impressive achievements in kinase inhibitor development there is a strong interest in development of *novel and selective* kinase inhibitors (including allosteric, covalent, bivalent) and subsequently qualitative kinases targeted libraries.

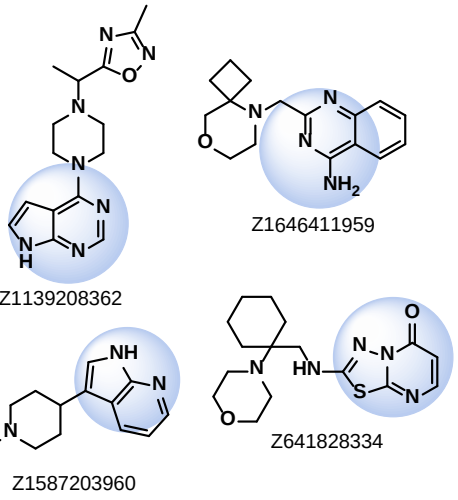
Our previous investigation and detailed structure analysis of known and most potent kinases' inhibitors yielded the complex approach to design of unique kinase focused libraries. We used several approaches with proven record in development of known successful kinase inhibitors. Validated *in silico* screening along with selection of compounds bearing privileged scaffolds/moieties and bioisosteric core

replacements were the key components of the dedicated deign. We also introduced carefully selected compounds that were similar to known drugs.

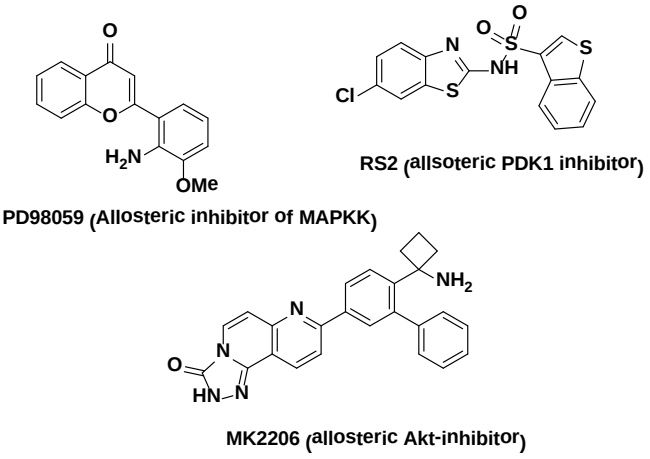
Hinge region directed sublibrary – 24,000 compounds



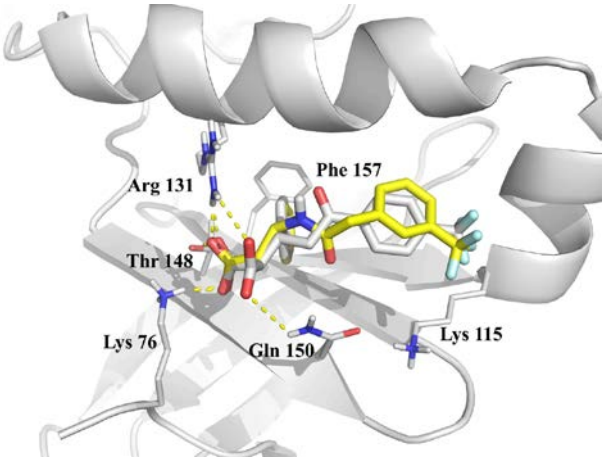
Well **validated Cores** with **New Chemistry decoration**



Pharmacophore & **Shape** similarity searches to the set of potent allosteric inhibitors



Docking into **allosteric kinases** binding sites



Docking calculations into **ATP-binding pocket**