All New Chemistry - Yours to Explore

## **Kinase Focused Library**

Protein kinases are among the most promising drug targets for anti-cancer treatment. The number of protein kinases encoded by the human genome is enormous, and there are plenty of inhibitors known to date, however, most of them have similar structures and selectivity issues.

The Life Chemicals Protein Kinase Focused Library comprises compounds selected from the Life Chemicals Stock Collection of Small Molecules for HTS by comparison to known kinase inhibitors. A reference set of 20,000 compounds with known kinase inhibitory activity extracted from ChEMBL database of bioactive molecules has been used for similarity search. Tanimoto similarity index of 0.85 was chosen as a search threshold. At the next stage, the substructure filters for detection and elimination of Pan Assay Interference (PAINS) compounds have been applied. As a result, around **30,000** compounds were selected for the Protein Kinase Focused Library.

Known inhibitors of the following protein kinases were used as a reference compound set for similarity search:

- 3-phosphoinositide dependent protein kinase-1
- Bcr/Abl fusion protein; Tyrosine-protein kinase ABL
- CaM kinase II delta
- CaM-kinase kinase beta; Serine/threonine-protein PIM3 PIM2 MAP kinase-interacting
- Casein kinase II
- Casein kinase II alpha
- c-Jun N-terminal kinase 1
- c-Jun N-terminal kinase 3
- Cyclin-dependent kinase 1; cyclin B1; cyclin H
- Cyclin-dependent kinase 1
- Cyclin-dependent kinase 2/cyclin A
- Cyclin-dependent kinase 2/cyclin E1
- Cyclin-dependent kinase 2
- Cyclin-dependent kinase 5/CDK5 activator 1
- Cyclin-dependent kinase 5/cyclin E1
- Cyclin-dependent kinase 7/ cyclin H
- Cyclin-dependent kinase 9
- Death-associated protein kinase 3
- Dual specificity mitogen-activated protein kinase 1
- Dual specificity protein kinase TTK
- Ephrin type-B receptor 4; Tyrosine-protein kinase SRC YES LCK
- Ephrin type-B receptor 4
- Epidermal growth factor receptor erbB1; and ErbB2 (HER1 HER2)
- Epidermal growth factor receptor erbB1; Receptor protein-tyrosine kinase erbB2
- Epidermal growth factor receptor erbB1; Receptor protein-tyrosine kinase erbB4
- Epidermal growth factor receptor erbB1



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- Glycogen synthase kinase-3; Cyclin-dependent kinase 5/CDK5 activator 1/cyclin B
- Glycogen synthase kinase-3
- Glycogen synthase kinase-3 alpha; beta
- Glycogen synthase kinase-3 alpha; Glycogen synthase kinase-3 beta
- Glycogen synthase kinase-3 beta
- Hepatocyte growth factor receptor
- Inhibitor of nuclear factor kappa B kinase beta subunit
- Insulin-like growth factor I receptor
- Leucine-rich repeat serine/threonine-protein kinase 2
- Macrophage colony stimulating factor
- MAP kinase p38 alpha
- MAP kinase p38 alpha; beta
- MAP kinase-activated protein kinase 2
- MAP kinase-interacting serine/threonine-protein kinase MNK1
- Mitogen-activated protein kinase 5
- Platelet-derived growth factor receptor
- Platelet-derived growth factor receptor beta
- Protein kinase C alpha
- Protein kinase C iota
- Protein kinase C mu
- Protein kinase C theta
- Protein kinase C zeta; iota
- Receptor protein-tyrosine kinase erbB2
- Rho-associated protein kinase 1
- Rho-associated protein kinase 2
- Serine/threonine-protein kinase 33
- Serine/threonine-protein kinase AKT
- Serine/threonine-protein kinase AKT2; Vascular endothelial growth factor receptor
- Serine/threonine-protein kinase AKT2
- Serine/threonine-protein kinase Aurora-A; Aurora-B
- Serine/threonine-protein kinase Aurora-A
- Serine/threonine-protein kinase B-raf
- Serine/threonine-protein kinase Chk1
- Serine/threonine-protein kinase Chk2
- Serine/threonine-protein kinase EEF2K
- Serine/threonine-protein kinase PIM1; Casein II alpha
- Serine/threonine-protein kinase PIM1
- Serine/threonine-protein kinase PIM2; PIM1
- Serine/threonine-protein kinase PIM2
- Serine/threonine-protein kinase PIM3; PIM1



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- Serine/threonine-protein kinase PIM3; PIM1 PIM2
- Serine/threonine-protein kinase RAF and Dual specificity mitogen-activated prote
- TGF-beta receptor type I
- TGF-beta receptor type II
- Tyrosine-protein kinase ABL; Bcr/Abl fusion protein
- Tyrosine-protein kinase ABL; SRC Epidermal growth factor receptor erbB1
- Tyrosine-protein kinase ABL
- Tyrosine-protein kinase FES; BMX ABL Fibroblast growth factor receptor 3
- Tyrosine-protein kinase JAK3; JAK2
- Tyrosine-protein kinase LCK; MAP p38 alpha
- Tyrosine-protein kinase LCK; Tyrosine non-receptor protein 2
- Tyrosine-protein kinase LCK
- Tyrosine-protein kinase receptor FLT3
- Tyrosine-protein kinase SRC; ABL Epidermal growth factor receptor erbB1
- Tyrosine-protein kinase SRC; Epidermal growth factor receptor erbB1
- Tyrosine-protein kinase SRC; Vascular endothelial growth factor receptor 2
- Tyrosine-protein kinase SRC
- Tyrosine-protein kinase TIE-2
- Vascular endothelial growth factor receptor
- Vascular endothelial growth factor receptor 1
- Vascular endothelial growth factor receptor 2