

imatinib

Ligand Id: 5687

Ligand name

imatinib

2D Structure

Cc1ccc(NC(=O)c2ccc(cc2)CN3CCNCC3)n4nc5ccncc5n4

Calculated Physico-chemical Properties

Hydrogen bond acceptors	8
Hydrogen bond donors	2
Rotatable bonds	8
Topological polar surface area	86.28
Molecular weight	493.26
XLogP	4.27
No. Lipinski's rules broken	0

Molecular properties generated using the CDK

SummaryBiological activityScreensClinical dataReferencesStructureSimilar ligands

Large-scale screening data

DiscoverRx kinome-wide affinity profile

Click on the image for a full-size view of the kinome-wide affinity profile for this compound.

Image was generated with the DiscoverRx TREEspot™ Compound Profile Visualization Software v4.0 using quantitative affinity data that were derived from the DiscoverRx KINOMEScan® platform.

To use the interactive DiscoverRx TREEspot™ Compound Profile Visualization Software, [click here](#).

DiscoverRx KINOMEScan® screen

A screen of 72 inhibitors against 456 human kinases. Quantitative data were derived using DiscoverRx KINOMEScan® platform.  
<http://www.discoverx.com/services/drug-discovery-development-services/kinase-profiling/kinomescan>  
Reference: 2,5

Key to terms and symbols

Click column headers to sort

Target	Name in screen	Sp.	Type	Action	Affinity	Units
discoidin domain receptor tyrosine kinase 1	DDR1	Hs	Inhibitor	Inhibition	9.1	p <i>K<sub>d</sub></i>
ABL proto-oncogene 1, non-receptor tyrosine kinase	ABL1-nonphosphorylated	Hs	Inhibitor	Inhibition	9.0	p <i>K<sub>d</sub></i>
ABL proto-oncogene 1, non-receptor tyrosine kinase	ABL1(Q252H)-nonphosphorylated	Hs	Inhibitor	Inhibition	8.7	p <i>K<sub>d</sub></i>
ABL proto-oncogene 1, non-receptor tyrosine kinase	ABL1(F317L)-nonphosphorylated	Hs	Inhibitor	Inhibition	8.6	p <i>K<sub>d</sub></i>
ABL proto-oncogene 1, non-receptor tyrosine kinase	ABL1(H396P)-nonphosphorylated	Hs	Inhibitor	Inhibition	8.2	p <i>K<sub>d</sub></i>
ABL proto-oncogene 1, non-receptor tyrosine kinase	ABL1(F317I)-nonphosphorylated	Hs	Inhibitor	Inhibition	8.1	p <i>K<sub>d</sub></i>
ABL proto-oncogene 2, non-receptor tyrosine kinase	ABL2	Hs	Inhibitor	Inhibition	8.0	p <i>K<sub>d</sub></i>
colony stimulating factor 1 receptor	CSF1R	Hs	Inhibitor	Inhibition	8.0	p <i>K<sub>d</sub></i>
v-kit Hardy-Zuckerman 4 feline sarcoma viral oncogene homolog	KIT	Hs	Inhibitor	Inhibition	7.9	p <i>K<sub>d</sub></i>
v-kit Hardy-Zuckerman 4 feline sarcoma viral oncogene homolog	KIT(L576P)	Hs	Inhibitor	Inhibition	7.8	p <i>K<sub>d</sub></i>

Displaying the top 10 targets    [View all targets in screen »](#)

EMD Millipore KinaseProfiler™ screen/Reaction Biology Kinase HotspotSM screen

A screen profiling 158 kinase inhibitors (Calbiochem Protein Kinase Inhibitor Library I and II, catalogue numbers 539744 and 539745) for their inhibitory activity at 1μM and 10μM against 234 human recombinant kinases using the EMD Millipore KinaseProfiler™ service.  
  
A screen profiling the inhibitory activity of 178 commercially available kinase inhibitors at 0.5μM against a panel of 300 recombinant protein kinases using the Reaction Biology Corporation Kinase HotspotSM platform.  
  
<http://www.millipore.com/techpublications/tech1/pf3036>  
<http://www.reactionbiology.com/webapps/main/pages/kinase.aspx>  
  
Reference: 1,3

Key to terms and symbols

Click column headers to sort

Target	Name in screen	Sp.	Type	Action	% Activity remaining at 0.5μM	% Activity remaining at 1μM	% Activity remaining at 10μM
platelet-derived growth factor receptor, alpha polypeptide	PDGFRα/PDGFRa	Hs	Inhibitor	Inhibition	5.9		
colony stimulating factor 1 receptor	Fms/FMS	Hs	Inhibitor	Inhibition	15.3		
discoidin domain receptor tyrosine kinase 2	DDR2/DDR2	Hs	Inhibitor	Inhibition	27.1		
LCK proto-oncogene, Src family tyrosine kinase	Lck/LCK	Hs	Inhibitor	Inhibition	30.9		
platelet-derived growth factor receptor, beta polypeptide	PDGFRβ/PDGFRb	Hs	Inhibitor	Inhibition	39.1		
ABL proto-oncogene 1, non-receptor tyrosine kinase	Abl/ABL1	Hs	Inhibitor	Inhibition	44.3		
Raf-1 proto-oncogene, serine/threonine kinase	c-RAF/RAF1	Hs	Inhibitor	Inhibition	47.9		
v-kit Hardy-Zuckerman 4 feline sarcoma viral oncogene homolog	cKit/c-Kit	Hs	Inhibitor	Inhibition	49.6		
ABL proto-oncogene 2, non-receptor tyrosine kinase	Arg/ABL2(ARG)	Hs	Inhibitor	Inhibition	55.9		
LYN proto-oncogene, Src family tyrosine kinase	Lyn/LYN	Hs	Inhibitor	Inhibition	59.6		

Displaying the top 10 targets    [View all targets in screen »](#)

**Supplementary Figure 1.** Display of the results of kinase inhibitor panel screening on a ligand page (under the “Screens” tab); an in-house curated IC<sub>50</sub> value from an individual publication is also included under the “Biological Activity” tab.