

Finding a potential inhibitor (Background)

- Increased gene expression leads to disease
- Research on KIT inhibitors can help drug discovery

The KIT protooncogene encodes for a receptor tyrosine kinase protein



Finding a potential inhibitor (1/11)

Go to the [PubChem homepage](#) and search for “[kit protooncogene](#)”:

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Explore Chemistry
Quickly find chemical information from authoritative sources

kit protooncogene

Compound	Gene
Protoanemonene	Sno oncogene
Delta(6)-protolludene	Raf oncogene
6-protolludene	Ret oncogene
Delta6-Protolludene	Mos oncogene
PROTOXIDE OF NITROGEN	Crk oncogene
Protoapigenone	ect2 oncogene
	MAS1 oncogene
	Pvt1 oncogene

Finding a potential inhibitor (2/11)

Click on the result, which will direct you to the gene summary page:

SEARCH FOR

kit protooncogene

Treating this as a text search.

Genes (1) **Literature** (142) **Patents** (11)

Searching gene targets tested in PubChem bioassays and those involved in PubChem pathways. [Read More...](#)

1 result

KIT - KIT proto-oncogene, receptor tyrosine kinase (human)

Gene ID: 3815 Gene Symbol: [KIT](#) Taxonomy: [Homo sapiens \(human\)](#)

Gene Synonyms: [KIT proto-oncogene, receptor tyrosine kinase](#); [C-Kit](#); [CD117](#); [MASTC](#); ...; [c-Kit protooncogene](#); ...

Linked BioAssays Count: [1,058](#) Linked Pathways Count: [34](#)

Source: Pathway, Patent

Finding a potential inhibitor (3/11)

Review fundamental information about the KIT protooncogene and navigate to the Contents table:

GENE SUMMARY

KIT - KIT proto-oncogene, receptor tyrosine kinase (human)

Cite Download

CONTENTS

Title and Summary

Names and Identifiers

Related Genes

Proteins

Chemicals and Bioactivities

BioAssays

Diseases and Phenotypes

Interactions and Pathways

Biochemical Reactions

Expression

Literature

Patents

Classification

Information Sources

Where can we find info on potential inhibitors? (Answer in Chat)

This gene encodes a receptor tyrosine kinase (KIT). The canonical form of this glycosylated transmembrane protein has an N-terminal extracellular region with five immunoglobulin-like domains, a transmembrane region, and an intracellular tyrosine kinase domain at the C-terminus. Upon activation by its cytokine ligand, stem cell factor (SCF), this protein phosphorylates multiple intracellular proteins that play a role in the proliferation, differentiation, migration and apoptosis of many cell types and thereby plays an important role in hematopoiesis, stem cell maintenance, gametogenesis, melanogenesis, and in mast cell development, migration and function. This protein can be a membrane-bound or soluble protein. Mutations in this gene are associated with gastrointestinal stromal tumors, mast cell disease, acute myelogenous leukemia, and piebaldism. Multiple transcript variants encoding different isoforms have been found for this gene. [provided by RefSeq, May 2020]

NCBI Gene

Finding a potential inhibitor (4/11)




Click on 4 Chemicals and Bioactivities and 4.1 Tested Compounds:

PubChem KIT - KIT proto-oncogene, receptor tyrosine kinase (human) (Gene)

4 Chemicals and Bioactivities

4.1 Tested Compounds

90,525 items View More Rows & Details Download

Structure	Activity	Activity Type	Activity Value, μM	Compound CID
	Active	Ki	0.000001	56593836
	Active	IC50	0.00002	130313537
	Active	Kd	0.000024	451705

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Finding a potential inhibitor (5/11)




Click Download to download the bioactivity data in CSV format:

PubChem KIT - KIT proto-oncogene, receptor tyrosine kinase (human) (Gene)

4 Chemicals and Bioactivities

4.1 Tested Compounds

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Structure	Activity	Activity Type	Activity Value, μM	Compound CID
	Active	Ki	0.000001	56593836
	Active	IC50	0.00002	130313537
	Active	Kd	0.000024	451705

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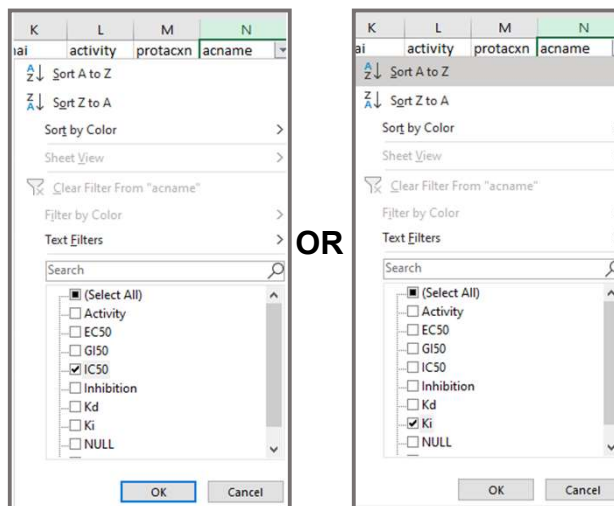
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Finding a potential inhibitor (6/11)

Open the CSV file:

- The CSV file contains more detailed information
- You can filter or order the dataset based on measures of inhibition (K_i or IC_{50} values) or substrate binding (K_D)



Finding a potential inhibitor (7/11)



Click View More Rows & Details for more information without downloading a file:

4 Chemicals and Bioactivities 🔍 🔗

4.1 Tested Compounds 🔍 🔗

90,525 Items View More Rows & Details Download




SORT BY Activity Value

Structure	Activity	Activity Type	Activity Value, μ M	Compound CID
	Active	Ki	0.000001	56593836
	Active	IC50	0.00002	130313537

Finding a potential inhibitor (8/11)

Sort Structures by Activity Value

SORT BY Activity Value ▾

#	Structure	Activity [?]	Activity Type [?]	Activity Value, μ M	Compound CID	Substance SID	BioAssay AID	BioAssay Name
1		Active	Ki					Displacement of [³³ P]ATP from human recombinant c-KIT domain after 20 mins by scintillation counting
2		Active	IC ₅₀					Inhibition of human c-KIT A loop exon 17 D820Y single mutant using poly (Glu,Tyr) 4:1 as substrate in presence of ³³ P-gamma-ATP by hotspot kinase assay
3		Active	Kd	0.000024	451705	50100119	1433	Kinase Inhibitor Selectivity Profiling Assay



Find a compound to learn more about!

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Finding a potential inhibitor (9/11)

Click on a relevant Compound CID for more information, including how to buy the compound:

SORT BY Activity Value ▾

#	Structure	Activity [?]	Activity Type [?]	Activity Value, μ M	Compound CID	Substance SID	BioAssay AID	BioAssay Name
1		Active	Ki	0.000001	56593836	134461981	623446	Displacement of [³³ P]ATP from human recombinant c-KIT domain after 20 mins by scintillation counting
2		Active	IC ₅₀	0.00002	130313537	440123730	1587963	Inhibition of human c-KIT A loop exon 17 D820Y single mutant using poly (Glu,Tyr) 4:1 as substrate in presence of ³³ P-gamma-ATP by hotspot kinase assay

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Finding a potential inhibitor (10/11)

Click on 5 Chemical Vendors:

COMPOUND SUMMARY

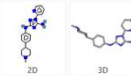
3-N-[4-(1-methylpiperidin-4-yl)phenyl]-1-pyridin-2-yl-1,2,4-triazole-3,5-diamine

99 Cite Download

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PubChem CID: 56593836

Structure:  2D 3D
Find Similar Structures

Molecular Formula: C₁₉H₂₃N₇

Synonyms: CHEMBL1835867, SCHEMBL4038099, BDBM50355489, ZINC72127621



Molecular Weight: 349.4


Dates: Modify: 2022-11-05, Create: 2012-02-06

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Finding a potential inhibitor (11/11)



Click on Purchasable Chemical ID for more information:



5 Chemical Vendors  


Showing 1 Substance per Vendor [View All](#)  [View in Entrez](#) [Download](#)

ZINC
PubChem SID: 330462129 **Purchasable Chemical: ZINC72127621**

PubChem

6 Patents  

6.1 Depositor-Supplied Patent Identifiers  

7 Items [View More Rows & Details](#)  [Download](#)

SORT BY: Priority Date

Publication Number	Title	Priority Date	Grant Date
EP-1562589-A2	Diaminotriazoles useful as inhibitors of protein kinases	2002-11-15	
EP-1562589-B1	Diaminotriazoles useful as inhibitors of protein kinases	2002-11-15	2009-01-07
KR-20060013480-A	Diaminotriazoles useful as inhibitors of protein kinases	2002-11-15	
US-2004214817-A1	Diaminotriazoles useful as inhibitors of protein kinases	2002-11-15	
US-2008014189-A1	Diaminotriazoles useful as inhibitors of protein kinases	2002-11-15	

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