Nilotinib is a second-generation inhibitor of the oncogenic tyrosine kinase BCR-ABL with IC$_{50}$ values of 19, 140, and 9,200 nM for wild-type, E255K, and T315I mutant forms of BCR-ABL, respectively (Kitagawa et al.; O’Hare; Verstovsek et al.). It binds to the ATP binding pocket of ABL, with higher affinity than Imatinib (Catalog #72532) (Manley et al. 2006; Verstovsek et al.). It also has activity below 1 µM against discoidin domain receptors (DDR) -1 and -2, platelet-derived growth factor receptors (PDGFR) -α and -β, stem cell factor receptor (c-KIT), and colony-stimulating factor 1 receptor (CSF-1R; Manley et al. 2010).

### Molecular Information
- **Chemical Name:** 4-methyl-N-[3-(4-methylimidazol-1-yl)-5-(trifluoromethyl)phenyl]-3-[(4-pyridin-3-ylpyrimidin-2-yl)amino]benzamide
- **Molecular Name:** Nilotinib
- **CAS Number:** 641571-10-0
- **Chemical Formula:** C$_{28}$H$_{22}$F$_{3}$N$_{7}$O$_{5}$
- **Molecular Weight:** 529.5 g/mol
- **Purity:** ≥ 95%
- **Chemical Name:** 4-methyl-N-[3-(4-methylimidazol-1-yl)-5-(trifluoromethyl)phenyl]-3-[(4-pyridin-3-ylpyrimidin-2-yl)amino]benzamide

### Properties
- **Physical Appearance:** A crystalline solid
- **Storage:** Product stable at -20°C as supplied. Protect from prolonged exposure to light. Stable as supplied for 12 months from date of receipt.
- **Solubility:**
  - DMSO ≤ 3.8 mM
  - For example, to prepare a 2 mM stock solution in DMSO, resuspend 10 mg in 9.4 mL of DMSO.

Prepare stock solution fresh before use. Information regarding stability of small molecules in solution has rarely been reported, however, as a general guide we recommend storage in DMSO at -20°C. Aliquot into working volumes to avoid repeated freeze-thaw cycles. The effect of storage of stock solution on compound performance should be tested for each application.

Compound has low solubility in aqueous media. For use as a cell culture supplement, stock solution should be diluted into culture medium immediately before use. Avoid final DMSO concentration above 0.1% due to potential cell toxicity.
Published Applications

MAINTENANCE AND SELF-RENEWAL
· Reduces fibrosis by promoting TNF-mediated apoptosis of mesenchymal stem cells (Lemos et al.).

CANCER RESEARCH
· Inhibits cellular proliferation in many wild-type and mutant forms of Philadelphia chromosome-positive acute lymphoblastic leukemia (Ph+ ALL) and chronic myeloid leukemia (CML) cells (O’Hare; Verstovsek et al.).
· Inhibits cell proliferation and progression through S phase in human lung cell line A549 through transcriptional changes in DNA helicase complex, cyclins, and cyclin-dependent kinases (Ji et al.).

References


Related Small Molecules

For a complete list of small molecules available from STEMCELL Technologies, visit www.stemcell.com/smallmolecules or contact us at techsupport@stemcell.com.

This product is hazardous. Please refer to the Safety Data Sheet (SDS).