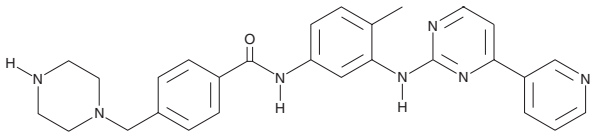
PRODUCT INFORMATION

N-desmethyl Imatinib

Item No. 16947

CAS Registry No.: 404844-02-6
Formal Name: N-[4-methyl-3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]-4-(1-piperazinylmethyl)-benzamide
Synonyms: N-desmethyl Gleevec, STI-509-00
MF: $C_{28}H_{29}N_7O$
FW: 479.6
Purity: ≥95%
UV/Vis.: λ_{max}: 237, 270 nm
Supplied as: A lyophilized solid
Storage: -20°C
Stability: ≥2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

N-desmethyl Imatinib is supplied as a lyophilized solid. A stock solution may be made by dissolving the N-desmethyl imatinib in the solvent of choice, which should be purged with an inert gas. N-desmethyl Imatinib is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of N-desmethyl imatinib in these solvents is approximately 0.2, 14, and 16 mg/ml, respectively.

N-desmethyl Imatinib is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, N-desmethyl imatinib should first be dissolved in DMF and then diluted with the aqueous buffer of choice. N-desmethyl Imatinib has a solubility of approximately 0.2 mg/ml in a 1:4 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

N-desmethyl Imatinib is a major active metabolite of imatinib (Item No. 13139), an anticancer agent that selectively targets tyrosine kinases, including Bcr-ABL, platelet-derived growth factor receptor (PDGFR), and KIT.[1,2] N-desmethyl Imatinib is formed when imatinib undergoes demethylation by the cytochrome P450 (CYP) isomer CYP3A4.[3] N-desmethyl Imatinib has the same *in vitro* potency at Bcr-ABL kinase as imatinib (IC_{50} = 38 nM for both) but is only present in plasma at 10-15% of the levels of imatinib, indicating the majority of the anticancer activity can be attributed to the parent compound.

References

1. Druker, B.J. Translation of the Philadelphia chromosome into therapy for CML. *Blood* **112(13)**, 4808-4817 (2008).
2. Müller, B.A. Imatinib and its successors-how modern chemistry has changed drug development. *Cur. Pharm. Des.* **15(2)**, 120-133 (2009).
3. Obach, R.S. Pharmacologically active drug metabolites: Impact on drug discovery and pharmacotherapy. *Pharmacol. Rev.* **65(2)**, 578-640 (2013).

CAYMAN CHEMICAL
1180 EAST ELLSWORTH RD
ANN ARBOR, MI 48108 · USA
PHONE: [800] 364-9897
[734] 971-3335
FAX: [734] 971-3640
CUSTSERV@CAYMANCHEM.COM
WWW.**CAYMANCHEM**.COM