

Certificate of Analysis

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Product Name: PX 12

Catalog No.: 2954

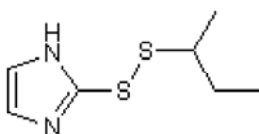
Batch No.: 1

CAS Number: 141400-58-0

IUPAC Name: 2-[(1-Methylpropyl)dithio]-1*H*-imidazole

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₇H₁₂N₂S₂
Batch Molecular Weight: 188.31
Physical Appearance: Cream solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.2 (Ethyl acetate:Petroleum ether [4:1])
HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Sulfur
Theoretical	44.65	6.42	14.88	34.05
Found	44.68	6.4	14.74	34.15

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Catalog No.: 2954

Batch No.: 1

CAS Number: 141400-58-0

IUPAC Name: 2-[(1-Methylpropyl)dithio]-1H-imidazole

Description:

PX 12 is a thioredoxin-1 (Trx-1) inhibitor; irreversibly inactivates Trx-1 as a substrate for reduction by thioredoxin reductase (TR); competitively inhibits the reduction of Trx-1 by TR ($K_i = 30.8 \mu\text{M}$). Attenuates expression of HIF-1 α , VEGF and iNOS (IC_{50} values are 7.2, 10.4 and 18.1 μM respectively). Exhibits antitumor activity; directly inhibits tubulin in vitro and decreases tumor microvessel density in vivo.

Physical and Chemical Properties:

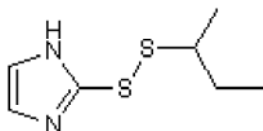
Batch Molecular Formula: $C_7H_{12}N_2S_2$

Batch Molecular Weight: 188.31

Physical Appearance: Cream solid

Minimum Purity: $\geq 99\%$

Batch Molecular Structure:



Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Jordan et al (2005) The thioredoxin-1 inhibitor 1-methylpropyl 2-imidazolyl disulfide (PX-12) decreases vascular permeability in tumor xenografts monitored by dynamic contrast enhanced magnetic resonance imaging. *Clin.Cancer Res.* **11** 529. PMID: 15701837.

Welsh et al (2003) The thioredoxin redox inhibitors 1-methylpropyl 2-imidazolyl disulfide and pleurotin inhibit hypoxia-induced factor 1 α and vascular endothelial growth factor formation. *Mol.Cancer.Ther.* **2** 235. PMID: 12657718.

Kirkpatrick et al (1998) Mechanisms of inhibition of the thioredoxin growth factor system by antitumor 2-imidazolyl disulfides. *Biochem.Pharmacol.* **55** 987. PMID: 9605422.

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