Print Date: Mar 23rd 2021

Certificate of Analysis

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Product Name: **(*S*)-ZINC 3573** **Catalog No.: 6352** **Batch No.: 1**

CAS Number: 2095596-11-3

IUPAC Name: (3*S*)-*N*,*N*-Dimethyl-1-(5-phenylpyrazolo[1,5-*a*]pyrimidin-7-yl)-3-pyrroldinamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{21}N_5$

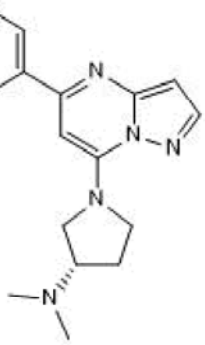
Batch Molecular Weight: 307.4

Physical Appearance: Off White solid

Solubility: 1eq. HCl to 100 mM
DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.49 (Dichloromethane:Methanol [4:1])

HPLC: Shows 99.7% purity

Chiral HPLC: Shows 99.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	70.33	6.89	22.78
Found	69.98	6.94	22.67

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

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Description:

(S)-ZINC 3573 is a negative control for (R)-ZINC 3573 (Cat. No. 6351). (S)-ZINC 3573 displays no activity at MRGPRX2 at concentrations below 100 µM.

Physical and Chemical Properties:

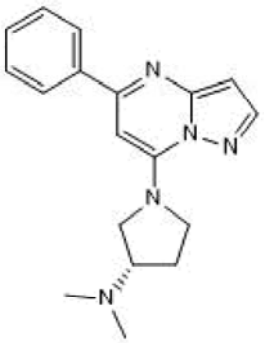
Batch Molecular Formula: $C_{18}H_{21}N_5$

Batch Molecular Weight: 307.4

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

1eq. HCl to 100 mM
DMSO to 100 mM
ethanol 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:

Lansu *et al* (2017) *In silico* design of novel probes for the atypical opioid receptor MRGPRX2. Nat.Chem.Biol. ***13*** 529. PMID: 28288109.