

Product Name: I-BRD9

Catalog No.: 5591

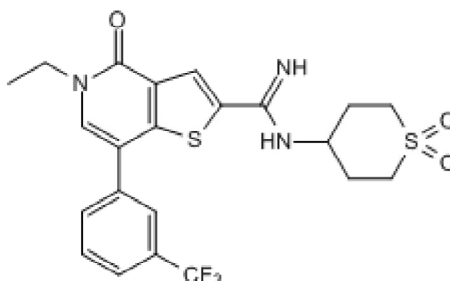
Batch No.: 4

CAS Number: 1714146-59-4

IUPAC Name: 5-Ethyl-4,5-dihydro-4-oxo-*N*-(tetrahydro-1,1-dioxido-2*H*-thiopyran-4-yl)-7-[3-(trifluoromethyl)phenyl]thieno[3,2-*c*]pyridine-2-carboximidamide

1. PHYSICAL AND CHEMICAL PROPERTIES

| | |
|-----------------------------------|---|
| Batch Molecular Formula: | C ₂₂ H ₂₂ F ₃ N ₃ O ₃ S ₂ . |
| Batch Molecular Weight: | 497.55 |
| Physical Appearance: | White solid |
| Solubility: | DMSO to 100 mM |
| Storage: | Store at -20°C |
| Batch Molecular Structure: | |



2. ANALYTICAL DATA

| | |
|---------------------------|---------------------------|
| HPLC: | Shows 98.1% purity |
| ¹H NMR: | Consistent with structure |
| Mass Spectrum: | Consistent with structure |

| | | | |
|-----------------------|--------------------------|------|------|
| Microanalysis: | Carbon Hydrogen Nitrogen | | |
| Theoretical | 53.11 | 4.46 | 8.45 |
| Found | 52.82 | 4.22 | 8.42 |

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

Product Name: I-BRD9

Catalog No.: 5591

4

CAS Number: 1714146-59-4

IUPAC Name: 5-Ethyl-4,5-dihydro-4-oxo-*N*-(tetrahydro-1,1-dioxido-2*H*-thiopyran-4-yl)-7-[3-(trifluoromethyl)phenyl]thieno[3,2-*c*]pyridine-2-carboximidamide

Description:

I-BRD9 is a potent and selective BRD9 inhibitor ($pI_{C_{50}} = 7.3$). Exhibits >70-fold selectivity for BRD9 over a panel of 34 other bromodomains and >700-fold selectivity over the BET family. Downregulates CLEC1, DUSP6, FES and SAMSN1 genes in Kasumi-1 cells.

Physical and Chemical Properties:

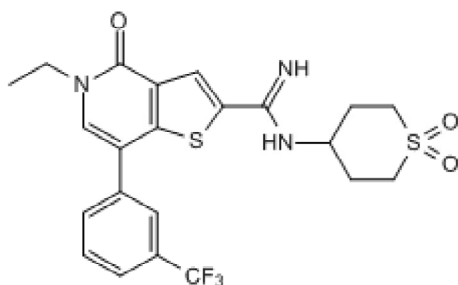
Batch Molecular Formula: C₂₂H₂₂F₃N₃O₃S₂.

Batch Molecular Weight: 497.55

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the I-BRD9 probe summary on the SGC website.

References:

Theodoulou *et al* (2015) Discovery of I-BRD9, a selective cell active chemical probe for bromodomain containing protein 9 inhibition. *J.Med.Chem* **59** 1425. PMID: 25856009.

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

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