

Product Name: I-BRD9

Catalog No.: 5591

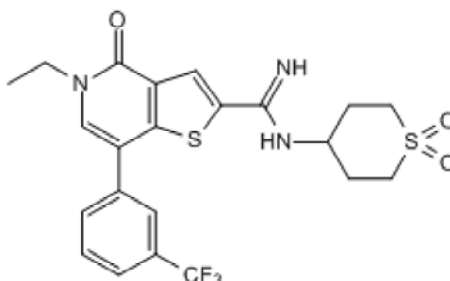
Batch No.: 3

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: C₂₂H₂₂F₃N₃O₃S₂
Batch Molecular Weight: 497.55
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.11	4.46	8.45
Found	53.02	4.56	8.33

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Description:

Potent and selective BRD9 inhibitor (pIC₅₀ = 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:

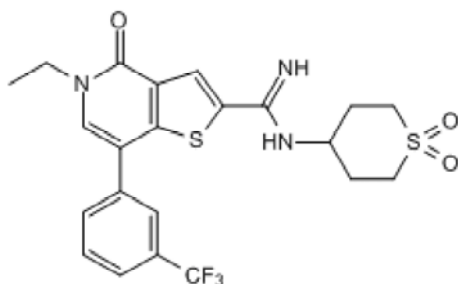
Batch Molecular Formula: C₂₂H₂₂F₃N₃O₃S₂

Batch Molecular Weight: 497.55

Physical Appearance: Off-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. 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.

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.

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