

Product Name: PFI 1

Catalog No.: 4445

Batch No.: 1

CAS Number: 1403764-72-6

IUPAC Name: 2-Methoxy-*N*-(3-methyl-2-oxo-1,2,3,4-tetrahydroquinazolin-6-yl)benzenesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₇N₃O₄S·¼H₂O

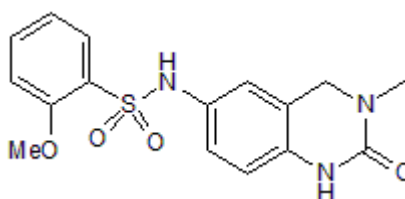
Batch Molecular Weight: 351.89

Physical Appearance: Beige solid

Solubility: DMSO to 50 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.15 (Chloroform:Methanol [95:5])

HPLC: Shows 98% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.61	5.01	11.94
Found	54.67	4.92	11.96

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Description:

Potent BET bromodomain inhibitor; exhibits inhibitory activity at bromodomain-containing protein (BRD) 2 and BRD4 (IC₅₀ values are 98 and 220 nM respectively). Induces apoptosis and G₁ cell cycle arrest in BET inhibitor-sensitive cell lines (MV4;11). Also downregulates Aurora B expression in MV4;11 cells. Cell permeable.

Physical and Chemical Properties:

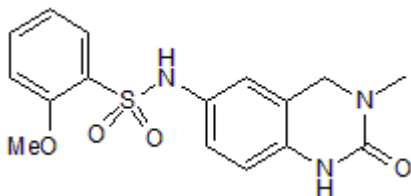
Batch Molecular Formula: C₁₆H₁₇N₃O₄S. ¼H₂O

Batch Molecular Weight: 351.89

Physical Appearance: Beige solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Fish et al (2012) Identification of a chemical probe for bromo and extra c-terminal bromodomain inhibition through optimization of a fragment-derived hit. *J.Med.Chem.* [Epub ahead of print]. PMID: 23095041.

Picaud et al (2013) PFI-1 - a highly selective protein interaction inhibitor targeting BET bromodomains. *Cancer Res.* [Epub ahead of print].

Storage: Store at RT

Solubility & Usage Info:

DMSO to 50 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.

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