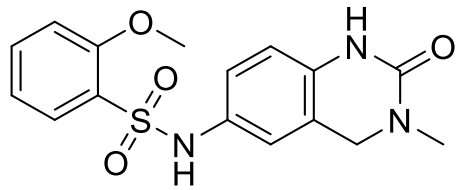
Product data sheet

MedKoo Cat#: 406261 Name: PFI-1 CAS: 1403764-72-6 Chemical Formula: $C_{16}H_{17}N_3O_4S$ Exact Mass: 347.0940 Molecular Weight: 347.389	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:

PFI-1 is a potent and highly selective protein interaction Inhibitor, which targets BET bromodomain. PFI-1 that efficiently blocks the interaction of BET BRDs with acetylated histone tails. Co-crystal structures showed that PFI-1 acts as an acetyl-lysine (Kac) mimetic inhibitor efficiently occupying the Kac binding site in BRD4 and BRD2. PFI-1 has antiproliferative effects on leukaemic cell lines and efficiently abrogates their clonogenic growth. Exposure of sensitive cell lines with PFI-1 results in G1 cell cycle arrest, down-regulation of MYC expression as well as induction of apoptosis and induces differentiation of primary leukaemic blasts.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMF	12.0	34.54
DMSO	32.93	94.78
DMSO:PBS (pH 7.2) (1:1)	0.5	1.44

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.88 mL	14.39 mL	28.79 mL
5 mM	0.58 mL	2.88 mL	5.76 mL
10 mM	0.29 mL	1.44 mL	2.88 mL
50 mM	0.06 mL	0.29 mL	0.58 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Picaud S, Da Costa D, Thanasopoulou A, Filippakopoulos P, Fish PV, Philpott M, Fedorov O, Brennan P, Bunnage ME, Owen DR, Bradner JE, Taniere P, O'Sullivan B, Müller S, Schwaller J, Stankovic T, Knapp S. PFI-1, a highly selective protein interaction inhibitor, targeting BET Bromodomains. Cancer Res. 2013 Jun 1;73(11):3336-46. doi: 10.1158/0008-5472.CAN-12-3292. Epub 2013 Apr 10. PMID: 23576556; PMCID: PMC3673830.

2. Fish PV, Filippakopoulos P, Bish G, Brennan PE, Bunnage ME, Cook AS, Federov O, Gerstenberger BS, Jones H, Knapp S, Marsden B, Nocka K, Owen DR, Philpott M, Picaud S, Primiano MJ, Ralph MJ, Sciammetta N, Trzupek JD. Identification of a chemical probe for bromo and extra C-terminal bromodomain inhibition through optimization of a fragment-derived hit. J Med Chem. 2012 Nov 26;55(22):9831-7. doi: 10.1021/jm3010515. Epub 2012 Nov 8. PMID: 23095041; PMCID: PMC3506127.

In vivo study

TBD

Product data sheet

7. Bioactivity

Biological target:

PFI-1 is a selective BET (bromodomain-containing protein) inhibitor for BRD4 with IC50 of 0.22 μM in a cell-free assay.

In vitro activity

PFI-1 has antiproliferative effects on leukemic cell lines and efficiently abrogates their clonogenic growth. Exposure of sensitive cell lines with PFI-1 results in G1 cell-cycle arrest, downregulation of MYC expression, as well as induction of apoptosis and induces differentiation of primary leukemic blasts. Intriguingly, cells exposed to PFI-1 showed significant downregulation of Aurora B kinase, thus attenuating phosphorylation of the Aurora substrate H3S10, providing an alternative strategy for the specific inhibition of this well-established oncology target.

Reference: Cancer Res. 2013 Jun 1;73(11):3336-46. https://pubmed.ncbi.nlm.nih.gov/23576556/

In vivo activity

TBD

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.