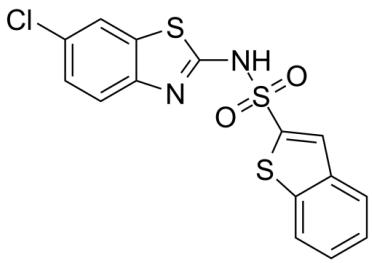
Data Sheet

Product Name:	PDK1-IN-RS2
Cat. No.:	CS-0063646
CAS No.:	1643958-89-7
Molecular Formula:	$C_{15}H_9ClN_2O_2S_3$
Molecular Weight:	380.89
Target:	PDK-1
Pathway:	PI3K/Akt/mTOR
Solubility:	DMSO : 125 mg/mL (328.18 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

PDK1-IN-RS2 is a mimic of peptide docking motif (PIFtide) and is a substrate-selective **PDK1** inhibitor with a K_d of 9 μM. PDK1-IN-RS2 suppresses the activation of the downstream kinases S6K1 by **PDK1**[1]. IC50 & Target: Kd: 9 μM (PDK1)[1] **In Vitro:** PDK1-IN-RS2 stimulates the catalytic activity of PDK1 toward a peptide substrate by sixfold. The sulfonyl group of PDK1-IN-RS2 interacts with Arg131 through a salt bridge, because the sulfonamide is likely ionized under the crystallization conditions[1].

References:

[1]. Rettenmaier TJ, et al. A small-molecule mimic of a peptide docking motif inhibits the protein kinase PDK1. Proc Natl Acad Sci U S A. 2014 Dec 30;111(52):18590-5.

CAIndexNames:

Benzo[b]thiophene-2-sulfonamide, N-(6-chloro-2-benzothiazolyl)-

SMILES:

O=S(C1=CC2=CC=CC=C2S1)(NC3=NC4=CC=C(C=C4S3)Cl)=O

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