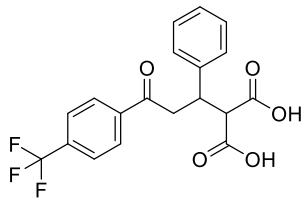
Product data sheet

MedKoo Cat#: 562629 Name: PS210 CAS#: 1221962-86-2 Chemical Formula: $C_{19}H_{15}F_3O_5$ Exact Mass: 380.0872 Molecular Weight: 380.31	
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:
PS210 is a substrate-selective inhibitor of protein kinase PDK1. It acts by binding to the PIF-pocket allosteric docking site.

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
DMSO	100	262.94

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.63 mL	13.15 mL	26.29 mL
5 mM	0.53 mL	2.63 mL	5.26 mL
10 mM	0.26 mL	1.31 mL	2.63 mL
50 mM	0.05 mL	0.26 mL	0.53 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

Busschots K, Lopez-Garcia LA, Lammi C, Stroba A, Zeuzem S, Piiper A, Alzari PM, Neimanis S, Arencibia JM, Engel M, Schulze JO, Biondi RM. Substrate-selective inhibition of protein kinase PDK1 by small compounds that bind to the PIF-pocket allosteric docking site. Chem Biol. 2012 Sep 21;19(9):1152-63. doi: 10.1016/j.chembiol.2012.07.017. PMID: 22999883.

In vivo study

TBD

7. Bioactivity
Biological target:

PS210 is a substrate-selective inhibitor of protein kinase PDK1.

Product data sheet

In vitro activity

The PIF-pocket of AGC protein kinases participates in the physiologic mechanism of regulation by acting as a docking site for substrates and as a switch for the transduction of the conformational changes needed for activation or inhibition. We describe the effects of compounds that bind to the PIF-pocket of PDK1. In vitro, PS210 is a potent activator of PDK1, and the crystal structure of the PDK1-ATP-PS210 complex shows that PS210 stimulates the closure of the kinase domain. However, in cells, the prodrug of PS210 (PS423) acts as a substrate-selective inhibitor of PDK1, inhibiting the phosphorylation and activation of S6K, which requires docking to the PIF-pocket, but not affecting PKB/Akt. This work describes a tool to study the dynamics of PDK1 activity and a potential approach for drug discovery.

Reference: Busschots K, Lopez-Garcia LA, Lammi C, Stroba A, Zeuzem S, Piiper A, Alzari PM, Neimanis S, Arencibia JM, Engel M, Schulze JO, Biondi RM. Substrate-selective inhibition of protein kinase PDK1 by small compounds that bind to the PIF-pocket allosteric docking site. Chem Biol. 2012 Sep 21;19(9):1152-63. doi: 10.1016/j.chembiol.2012.07.017. PMID: 22999883.

In vivo activity

TBD