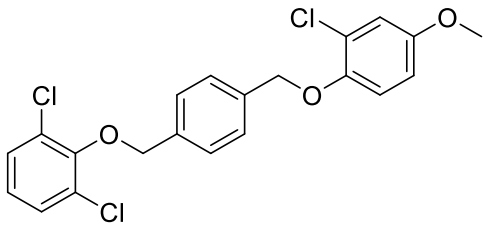
Product data sheet

MedKoo Cat#: 319719 Name: Pocapavir CAS#: 146949-21-5 Chemical Formula: $C_{21}H_{17}Cl_3O_3$ Exact Mass: 422.0243 Molecular Weight: 423.714	
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:
Pocapavir, also known as SCH-48973 and V-073, is a potent, selective, antienterovirus agent. SCH-48973 had antiviral activity (50% inhibitory concentrations [IC50s]) of 0.02 to 0.11 microg/ml, with no detectable cytotoxicity at 50 microg/ml. SCH-48973 inhibited 80% of 154 recent human enterovirus isolates at an IC50 of 0.9 microg/ml. The affinity constant (Ki) for SCH-48973 binding to poliovirus was 8.85 x 10(-8) M. SCH-48973 demonstrated efficacy in a murine poliovirus model of enterovirus disease. SCH-48973 represents a potential candidate for therapeutic intervention against enterovirus infections.

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	236.00

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.36 mL	11.80 mL	23.60 mL
5 mM	0.47 mL	2.36 mL	4.72 mL
10 mM	0.24 mL	1.18 mL	2.36 mL
50 mM	0.05 mL	0.24 mL	0.47 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. Oberste MS, Moore D, Anderson B, Pallansch MA, Pevear DC, Collett MS. In vitro antiviral activity of V-073 against polioviruses. Antimicrob Agents Chemother. 2009 Oct;53(10):4501-3. doi: 10.1128/AAC.00671-09. Epub 2009 Jul 27. PMID: 19635956; PMCID: PMC2764203.

2. Buontempo PJ, Cox S, Wright-Minogue J, DeMartino JL, Skelton AM, Ferrari E, Albin R, Rozhon EJ, Girijavallabhan V, Modlin JF, O'Connell JF. SCH 48973: a potent, broad-spectrum, antienterovirus compound. Antimicrob Agents Chemother. 1997 Jun;41(6):1220-5. doi: 10.1128/AAC.41.6.1220. PMID: 9174174; PMCID: PMC163890.

In vivo study

1. Buontempo PJ, Cox S, Wright-Minogue J, DeMartino JL, Skelton AM, Ferrari E, Albin R, Rozhon EJ, Girijavallabhan V, Modlin JF, O'Connell JF. SCH 48973: a potent, broad-spectrum, antienterovirus compound. Antimicrob Agents Chemother. 1997 Jun;41(6):1220-5. doi: 10.1128/AAC.41.6.1220. PMID: 9174174; PMCID: PMC163890.

7. Bioactivity

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Biological target:

Pocapavir (SCH-48973, V-073) is an inhibitor of investigational enterovirus (EV) capsid.

In vitro activity

To assess the spectrum of antipoliovirus activity of V-073, a panel of 45 polioviruses was assembled and evaluated in a cell culture cytopathic effect assay. The panel consisted of viruses from all three poliovirus serotypes and included wild reference strains. The assay for drug susceptibility measured protection by the drug of an LLC-MK2 cell monolayer from the virus replication-induced cytopathic effect. The 50% effective concentration (EC50) values for the 45 individual viruses, as determined from seven-point concentration curves using a four-parameter curve-fitting program (SoftMax Pro; Molecular Devices), are provided in Table 1. V-073 was active against all viruses in this panel, with EC50s ranging from 0.003 μM to 0.126 μM. The distribution of drug susceptibilities among these 45 polioviruses is depicted in Fig. 2. Ninety percent of all polioviruses tested were inhibited by V-073 at EC50s of ⩽ 0.076 μM (MIC90 = 76 nM; 32 ng/ml). In Table Table2,2, the mean EC50s for the various categories of polioviruses are provided. There appears to be no bias in the activity of V-073 among these virus groupings.

Reference: Antimicrob Agents Chemother. 2009 Oct;53(10):4501-3. https://www.ncbi.nlm.nih.gov/pmc/articles/pmid/19635956/

In vivo activity

For mice infected with poliovirus type 2 and treated (beginning either 6 or 24 h after infection) with SCH 48973 at 20 mg/kg/day, there was a significant reduction (1 to 2 logs) in the titer of virus recovered from the brains 2 days after infection (Table 2). The difference between the two regimens (6 and 24 h) was not significant. When brains from noninfected, SCH 48973-treated mice were removed, homogenized, diluted, and inoculated in vitro with known quantities of virus, no reduction of viral plaques compared to the input inoculum was observed (data not shown). These results indicate that the reduction in viral load in brains is due to a direct effect of SCH 48973 in vivo and not due to compound carryover into the tissue culture system.

Reference: Antimicrob Agents Chemother. 1997 Jun;41(6):1220-5. https://www.ncbi.nlm.nih.gov/pmc/articles/pmid/9174174/