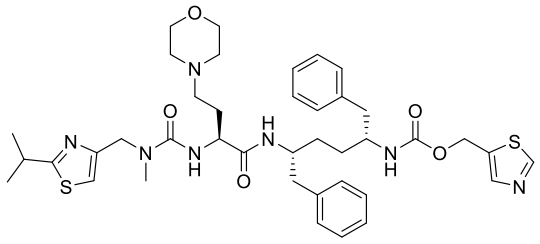
Product data sheet

MedKoo Cat#: 300151 Name: Cobicistat CAS#: 1004316-88-4 Chemical Formula: $C_{40}H_{53}N_7O_5S_2$ Exact Mass: 775.35496 Molecular Weight: 776.02	
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:

Cobicistat, also known as GS9350, is an approved drug for use in the treatment of infection with the human immunodeficiency virus (HIV). Like ritonavir (Norvir), cobicistat is of interest not for its anti-HIV properties, but rather its ability to inhibit liver enzymes that metabolize other medications used to treat HIV, notably elvitegravir, an HIV integrase inhibitor currently under investigation itself. By combining cobicistat with elvitegravir, higher concentrations of elvitgravir are achieved in the body with lower dosing, theoretically enhancing elvitgravir's viral suppression while diminishing its adverse side-effects. In contrast with ritonavir, the only currently approved booster, cobicistat has no anti-HIV activity of its own. Cobicistat is a component of the four-drug, fixed-dose combination HIV treatment elvitegravir/cobicistat/emtricitabine/tenofovir (known as the "Quad Pill"). The Quad Pill was approved by the FDA in August 2012 for use in the United States and is owned by Gilead Sciences.

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	106.67	137.46
DMSO:PBS (pH 7.2) (1:1)	0.5	0.64
DMF	20.0	25.77
Ethanol	55.0	70.87

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	1.29 mL	6.44 mL	12.89 mL
5 mM	0.26 mL	1.29 mL	2.58 mL
10 mM	0.13 mL	0.64 mL	1.29 mL
50 mM	0.03 mL	0.13 mL	0.26 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. Xu L, Liu H, Murray BP, Callebaut C, Lee MS, Hong A, Strickley RG, Tsai LK, Stray KM, Wang Y, Rhodes GR, Desai MC. Cobicistat (GS-9350): A Potent and Selective Inhibitor of Human CYP3A as a Novel Pharmacoenhancer. ACS Med Chem Lett. 2010 May 17;1(5):209-13. doi: 10.1021/ml1000257. PMID: 24900196; PMCID: PMC4007915.

In vivo study

TBD

Product data sheet

7. Bioactivity

Biological target:

Cobicistat is an inhibitor of cytochrome P450 3A (CYP3A) enzymes with IC50s of 30-285 nM.

In vitro activity

The mode of inhibition of human CYP3A by compound 3 (cobicistat) was extensively compared with that of RTV. Similar to RTV, 3 inhibitory effects on CYP3A may involve direct interaction and mechanism-based inhibition. Besides interacting directly at the heme group of the CYP3A enzyme, 3 is also an effective mechanism-based inhibitor of CYP3A with an inhibitory potency dependent upon its metabolism. Importantly, compound 3 and RTV inactivate CYP3A similarly at both low and high concentrations and in a time- and concentration-dependent manner. The corresponding estimates of kinact and KI are presented in Table 2. These results suggest that RTV and 3 share the same mechanism of action for the inhibition of CYP3A.

Reference: ACS Med Chem Lett. 2010 Aug 12; 1(5): 209–213. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4007915/

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.