# **Product data sheet**



MedKoo Cat#: 565615				
Name: OD36 hydrochloride		CI /		
CAS: 1638644-62-8				
Chemical Formula: C <sub>16</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>2</sub>				
Exact Mass: 366.065				
Molecular Weight: 367.23		HCI		
Product supplied as:	Powder			
Purity (by HPLC):	≥ 98%			
Shipping conditions	Ambient temperature	NH O		
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.			
_	In solvent: -80°C 3 months; -20°C 2 weeks.			

#### 1. Product description:

OD36 hydrochloride is a novel potent and selective receptor-interacting protein kinase 2 (ripk2) inhibitor

### 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	35.03	95.38
Ethanol	1.84	5.01

#### 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.02 mL	15.12 mL	30.23 mL
5 mM	0.60 mL	3.02 mL	6.05 mL
10 mM	0.30 mL	1.51 mL	3.02 mL
50 mM	0.06 mL	0.30 mL	0.60 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

Tigno-Aranjuez JT, Benderitter P, Rombouts F, Deroose F, Bai X, Mattioli B, Cominelli F, Pizarro TT, Hoflack J, Abbott DW. In vivo inhibition of RIPK2 kinase alleviates inflammatory disease. J Biol Chem. 2014 Oct 24;289(43):29651-64. doi: 10.1074/jbc.M114.591388. Epub 2014 Sep 11. PMID: 25213858; PMCID: PMC4207980.

#### In vivo study

Tigno-Aranjuez JT, Benderitter P, Rombouts F, Deroose F, Bai X, Mattioli B, Cominelli F, Pizarro TT, Hoflack J, Abbott DW. In vivo inhibition of RIPK2 kinase alleviates inflammatory disease. J Biol Chem. 2014 Oct 24;289(43):29651-64. doi: 10.1074/jbc.M114.591388. Epub 2014 Sep 11. PMID: 25213858; PMCID: PMC4207980.

## 7. Bioactivity

Biological target:

OD36 is a RIPK2 inhibitor with an IC50 of 5.3 nM.

#### In vitro activity

The most potent compound (OD36) and Gefitinib were profiled against 366 kinases, whereas OD38 was screened against 88 kinases. The kinase profiles, visualized as dendrograms, and the extent of inhibition are graphically represented in Fig. 3A. At 100 nm, both OD36 and OD38 show very good initial specificity, inhibiting few other kinases to the same extent as RIPK2 and showing very high

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potency with IC<sub>50</sub> values in the lower nanomolar range (OD36 having an IC<sub>50</sub> of 5.3 nm and OD38 having an IC<sub>50</sub> of 14.1 nm, Fig. 3A).

Reference: J Biol Chem. 2014 Oct 24;289(43):29651-64. https://pubmed.ncbi.nlm.nih.gov/25213858/

#### In vivo activity

As shown in Fig. 5A, both Gefitinib and OD36 inhibited the recruitment of inflammatory cells to the peritoneum, specifically that of neutrophils, and, to a lesser extent, lymphocytes. Statistical analysis of peritoneal lavage cell subsets shows a significant effect of both Gefitinib and OD36 in inhibiting MDP-induced peritonitis (Fig. 5B). Although there was quite some variability between animals, for a number of analytes tested, there was also an observable trend in decrease of secreted chemokines in either the Gefitinib or in the OD36-treated mice (supplemental Fig. S3). These very promising in vivo results for an early-stage RIPK2 inhibitor such as OD36, which also shows potent in vitro activity and good initial selectivity, encourages continued optimization of such RIPK2 inhibitors that will retain potency but in addition display enhanced specificity and an improved half-life in vivo.

Reference: J Biol Chem. 2014 Oct 24;289(43):29651-64. https://pubmed.ncbi.nlm.nih.gov/25213858/

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.