

Product Name: OD 36 hydrochloride

Catalog No.: 6598

Batch No.: 1

CAS Number: 1638644-62-8

IUPAC Name: 6-Chloro-10,11,14,17-tetrahydro-13*H*-1,16-etheno-4,8-metheno-1*H*-pyrazolo[3,4-*g*][1,14,4,6]dioxadiazacyclohexadecine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₅ClN₄O₂.HCl.¼H₂O

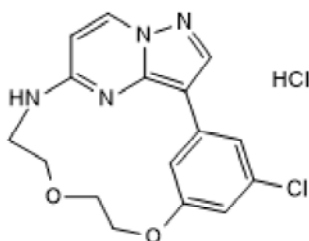
Batch Molecular Weight: 371.73

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.7	4.47	15.07
Found	51.91	4.46	14.73

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Description:

Potent receptor-interacting protein kinase 2 (RIPK2) inhibitor (IC_{50} = 5.3 nM). Displays similar % inhibition against ALK-2 and SIK2 at 100 nM. Downregulates expression of a panel of RIPK2-dependent genes. Inhibits recruitment of inflammatory cells in a mouse MDP-induced peritonitis model.

Physical and Chemical Properties:

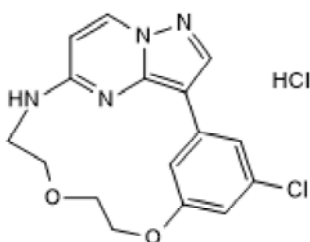
Batch Molecular Formula: $C_{16}H_{15}ClN_4O_2 \cdot HCl \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 371.73

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Tigno-Aranjuez et al (2014) *In vivo* inhibition of RIPK2 kinase alleviates inflammatory disease. *J.Biol.Chem.* **289** 29651. PMID: 25213858.

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