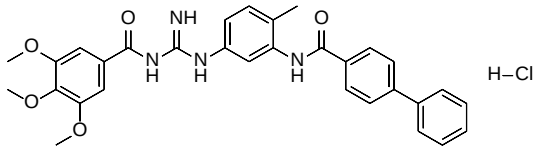
Product data sheet

MedKoo Cat#: 407238 Name: MRT-83 HCl salt CAS: 1359944-60-7 (HCl) Chemical Formula: $C_{31}H_{31}ClN_4O_5$ Molecular Weight: 575.062	
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:

MRT-83 is a novel potent antagonist of Smo. MRT-83 blocks Hedgehog (Hh) signaling in various assays with an IC50 in the nanomolar range, showing greater potency than the reference Smo antagonist cyclopamine. MRT-83 inhibits Bodipy-cyclopamine binding to human and mouse Smo. MRT-83 abrogates the agonist-induced trafficking of endogenous mouse or human Smo to the primary cilium of C3H10T1/2 or NT2 cells that derive from a pluripotent testicular carcinoma. MRT-83 efficiently antagonizes Hh signaling in vivo. MRT-83 will be useful for manipulating Hh signaling and may help develop new therapies against Hh-pathway related diseases.

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	250.0	434.74

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.74 mL	8.69 mL	17.39 mL
5 mM	0.35 mL	1.74 mL	3.48 mL
10 mM	0.17 mL	0.87 mL	1.74 mL
50 mM	0.04 mL	0.17 mL	0.35 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

Roudaut H, Traiffort E, Gorojankina T, Vincent L, Faure H, Schoenfelder A, Mann A, Manetti F, Solinas A, Taddei M, Ruat M. Identification and mechanism of action of the acylguanidine MRT-83, a novel potent Smoothened antagonist. Mol Pharmacol. 2011 Mar;79(3):453-60. doi: 10.1124/mol.110.069708. Epub 2010 Dec 21. PMID: 21177415.

In vivo study

Roudaut H, Traiffort E, Gorojankina T, Vincent L, Faure H, Schoenfelder A, Mann A, Manetti F, Solinas A, Taddei M, Ruat M. Identification and mechanism of action of the acylguanidine MRT-83, a novel potent Smoothened antagonist. Mol Pharmacol. 2011 Mar;79(3):453-60. doi: 10.1124/mol.110.069708. Epub 2010 Dec 21. PMID: 21177415.

7. Bioactivity

Biological target:

MRT-83 (hydrochloride) is the potent antagonist of Smoothened (Smo) receptor.

In vitro activity

Product data sheet

MRT-83 blocks Hedgehog (Hh) signaling in various assays with an IC50 in the nanomolar range, showing greater potency than the reference Smo antagonist cyclopamine. MRT-83 inhibits Bodipy-cyclopamine binding to human and mouse Smo but does not modify Wnt signaling in human embryonic kidney 293 transiently transfected with a Tcf/Lef-dependent Firefly luciferase reporter together with a Renilla reniformis luciferase control reporter.

Reference: Mol Pharmacol. 2011 Mar;79(3):453-60. https://pubmed.ncbi.nlm.nih.gov/21177415/

In vivo activity

MRT-83 abrogates the agonist-induced trafficking of endogenous mouse or human Smo to the primary cilium of C3H10T1/2 or NT2 cells that derive from a pluripotent testicular carcinoma. Stereotaxic injection into the lateral ventricle of adult mice of MRT-83 but not of a structurally related compound inactive at Smo abolished up-regulation of Patched transcription induced by Sonic Hedgehog in the neighboring subventricular zone. These data demonstrate that MRT-83 efficiently antagonizes Hh signaling in vivo.

Reference: Mol Pharmacol. 2011 Mar;79(3):453-60. https://pubmed.ncbi.nlm.nih.gov/21177415/