# **Product data sheet**



MedKoo Cat#: 206503					
Name: Theliatinib free base					
CAS: 1353644-70-8 (free base)					
Chemical Formula: C <sub>25</sub> H <sub>26</sub> N <sub>6</sub> O <sub>2</sub>					
Exact Mass: 442.2117					
Molecular Weight: 442.52					
Product supplied as: Powder					
Purity (by HPLC): $\geq 98\%$					
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:

Theliatinib, also known as xiliertinib and HMPL-309, is a novel small molecule, epidermal growth factor receptor tyrosine kinase inhibitor with potential antineoplastic and anti-angiogenesis activities. In vitro studies suggest that Theliatinib is a potent EGFR kinase inhibitor with good kinase selectivity and in vivo data demonstrated broad spectrum anti-tumor activity via oral dosing in multiple xerographs such as A-431, Bcap-37 and Fadu.

## 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	47	106.21

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.26 mL	11.30 mL	22.60 mL
5 mM	0.45 mL	2.26 mL	4.52 mL
10 mM	0.23 mL	1.13 mL	2.26 mL
50 mM	0.05 mL	0.23 mL	0.45 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

To be determined

## In vivo study

 Ren Y, Zheng J, Fan S, Wang L, Cheng M, Shi D, Zhang W, Tang R, Yu Y, Jiao L, Ni J, Yang H, Cai H, Yin F, Chen Y, Zhou F, Zhang W, Qing W, Su W. Anti-tumor efficacy of theliatinib in esophageal cancer patient-derived xenografts models with epidermal growth factor receptor (EGFR) overexpression and gene amplification. Oncotarget. 2017 Apr 19;8(31):50832-50844. doi: 10.18632/oncotarget.17243. PMID: 28881608; PMCID: PMC5584209.

## 7. Bioactivity

Biological target:

Theliatinib is an EGFR inhibitor with a Ki of 0.05 nM and an IC50 of 3 nM. Theliatinib has an IC50 of 22 nM for the EGFR T790M/L858R mutant. Theliatinib shows >50-fold selectivity for EGFR than other kinases.

In vitro activity

To be determined

# **Product data sheet**



In vivo activity

Theliatinib could potentially benefit esophageal cancer (EC) patients with high EGFR protein expression without mutations or abnormal activities of associated factors, such as PI3KCA or FGFR1. Theliatinib exhibited strong antitumor activity in patient-derived EC xenograft (PDECX) models with high EGFR expression, including substantial tumor regression in two PDECX models with both EGFR gene amplification and protein overexpression.

Reference: Oncotarget. 2017 Apr 19;8(31):50832-50844. https://pubmed.ncbi.nlm.nih.gov/28881608/

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.