# HET0016

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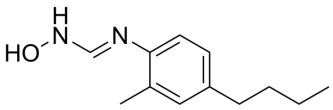
| **Cat. No.:** | HY-124527 |
| **CAS No.:** | 339068-25-6 |
| **Molecular Formula:** | $C_{12}H_{18}N_2O$ |
| **Molecular Weight:** | 206.28 |
| **Target:** | Cytochrome P450 |
| **Pathway:** | Metabolic Enzyme/Protease |
| **Storage:** | Powder -20°C 3 years<br>4°C 2 years<br>In solvent -80°C 2 years<br>-20°C 1 year |



## SOLVENT & SOLUBILITY

**In Vitro**

DCM : 12.5 mg/mL (60.60 mM; Need ultrasonic)
DMSO : 5 mg/mL (24.24 mM; Need ultrasonic)

**Preparing Stock Solutions**

| Solvent / Mass / Concentration | 1 mg | 5 mg | 10 mg |
|---|---|---|---|
| 1 mM | 4.8478 mL | 24.2389 mL | 48.4778 mL |
| 5 mM | 0.9696 mL | 4.8478 mL | 9.6956 mL |
| 10 mM | 0.4848 mL | 2.4239 mL | 4.8478 mL |

Please refer to the solubility information to select the appropriate solvent.

**In Vivo**

1. Add each solvent one by one: 20% HP-β-CD in saline
   Solubility: 2 mg/mL (9.70 mM); Clear solution; Need ultrasonic

## BIOLOGICAL ACTIVITY

**Description**

HET0016 is a potent and selective 20-hydroxyeicosatetraenoic acid (20-HETE) synthase inhibitor, with $IC_{50}$ values of 17.7 nM, 12.1 nM and 20.6 nM for recombinant CYP4A1-, CYP4A2- and CYP4A3-catalyzed 20-HETE synthesis, respectively. HET0016 also is a selective CYP450 inhibitor, which has been shown to inhibit angiogenesis and tumor growth[1][2].

**$IC_{50}$ & Target**

CYP4

**In Vitro**

HET0016 is a selective, non-competitive and irreversible inhibitor of CYP4A [1].
HET0016 (100 μM; 24 hours, 48 hours) decreases migration and invasion of breast cancer metastatic cells [2].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Proliferation Assay[2]

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| Cell Line: | MDA-MB-231 cells |
| Concentration: | 100 μM |
| Incubation Time: | 24 hours, 48 hours |
| Result: | Decreased migration and invasion of breast cancer metastatic cells |

**In Vivo**

HET0016 (10 mg/kg/day; i.v.; for 3 weeks) reduces tumor volume and lung metastasis in an immunocompetent breast cancer mouse model[2].
HET0016 reduces the metalloproteinases' levels in the lungs via PI3K/AKT pathway in mice[2].
HET0016 decreases expression of pro-inflammatory and growth factors and granulocytic MDSCs population in lung microenvironment[2].
HET0016 protects BBB dysfunction after I/R by regulating the expression of MMP-9 and tight junction proteins[3].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

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| Animal Model: | 4–5 weeks female Balb/c mice (16-18 g)[2] |
| Dosage: | 10 mg/kg/day |
| Administration: | Intravenously; 5 days a week; for 3 weeks; starting from day 15 of tumor implantation |
| Result: | Reduced tumor volume and lung metastasis. |

## CUSTOMER VALIDATION

- Cell Death Dis. 2022 Jul 28;13(7):653.
- Neuropharmacology. 2023 Aug 12;239:109687.

See more customer validations on www.MedChemExpress.com

## REFERENCES

[1]. Seki T, et al. Cytochrome P450 4A isoform inhibitory profile of N-hydroxy-N'-(4-butyl-2-methylphenyl)-formamidine (HET0016), a selective inhibitor of 20-HETE synthesis. Biol Pharm Bull. 2005 Sep;28(9):1651-4.

[2]. Borin TF, et al. HET0016 decreases lung metastasis from breast cancer in immune-competent mouse model. PLoS One. 2017 Jun 13;12(6):e0178830.

[3]. Liu Y, et al. The protective effect of HET0016 on brain edema and blood-brain barrier dysfunction after cerebral ischemia/reperfusion. Brain Res. 2014 Jan 28;1544:45-53.



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