# RORγt inverse agonist 13

**Cat. No.:** HY-131338

**CAS No.:** 2170477-75-3

**Molecular Formula:** $C_{23}H_{17}Cl_2F_3N_2O_4$

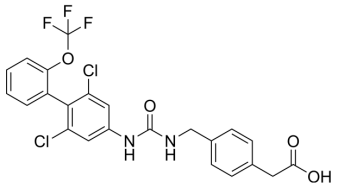
**Molecular Weight:** 513.29

**Target:** ROR

**Pathway:** Metabolic Enzyme/Protease; Vitamin D Related/Nuclear Receptor

**Storage:**

| | | |
|---|---|---|
| Powder | -20°C | 3 years |
| In solvent | -80°C | 6 months |
| | -20°C | 1 month |



## SOLVENT & SOLUBILITY

**In Vitro**

DMSO : 100 mg/mL (194.82 mM; Need ultrasonic)

| Preparing Stock Solutions | Solvent / Mass / Concentration | 1 mg | 5 mg | 10 mg |
|---|---|---|---|---|
| | 1 mM | 1.9482 mL | 9.7411 mL | 19.4822 mL |
| | 5 mM | 0.3896 mL | 1.9482 mL | 3.8964 mL |
| | 10 mM | 0.1948 mL | 0.9741 mL | 1.9482 mL |

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

**In Vivo**

1. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.87 mM); Clear solution

## BIOLOGICAL ACTIVITY

**Description**

RORγt inverse agonist 13 (Compound 3i) is a potent, orally active and selective RORγt inverse agonist, with improved agent-like properties, with an $IC_{50}$ of 63.8 nM[1].

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

ROR-γ
63.8 nM ($IC_{50}$)

**In Vitro**

RORγt inverse agonist 13 (Compound 3i) exhibits activity with an inhibition of 76% at 0.3 μM in Th17 cell differentiation assay [1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

**In Vivo**

RORγt inverse agonist 13 (Compound 3i, 25 mg/kg, Orally, twice daily) demonstrats excellent in vivo PK profile in mice and good in vivo efficacy in an IMQ-induced psoriasis mice model[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

| | |
|---|---|
| Animal Model: | Imiquimod (IMQ)-induced psoriasis mice model[1]. |
| Dosage: | 25 mg/kg. |
| Administration: | Orally, twice daily. |
| Result: | Brought in a significant reduction in clinical severity of psoriasis as measured through the ear erythema, back skin erythema and scaliness scales. |

| | |
|---|---|
| Animal Model: | Male CD-1 Mice[1]. |
| Dosage: | 1 mg/kg (i.v.) and 5 mg/kg (p.o.)(Pharmacokinetic Analysis). |
| Administration: | IV or PO, single dose. |
| Result: | $C_{max}$: 609.67 ng/mL (PO), 1550 ng/mL (IV).<br>$T_{1/2}$: 3.63 h (PO), 3.04 h (IV). |

## REFERENCES

[1]. Nannan Sun, et al. Discovery of carboxyl-containing biaryl ureas as potent RORγt inverse agonists. Eur J Med Chem. 2020 Jul 5;202:112536.



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