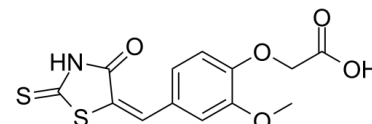


Data Sheet

Product Name:	IMR-1A
Cat. No.:	CS-5752
CAS No.:	331862-41-0
Molecular Formula:	C ₁₃ H ₁₁ NO ₅ S ₂
Molecular Weight:	325.36
Target:	Drug Metabolite; Notch
Pathway:	Metabolic Enzyme/Protease; Neuronal Signaling; Stem Cell/Wnt
Solubility:	DMSO : 2 mg/mL (6.15 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

IMR-1A, a acid metabolite of IMR-1, is a **Notch** inhibitors with an **IC₅₀** of 0.5 μM. IMR-1A has a 50-fold increase in potency with respect to IMR-1. IMR-1 can metabolize in vivo to IMR-1A^[1]. **IC₅₀ & Target:** IC₅₀: 0.5 μM (Notch)^[1] **In Vivo:** IMR-1A (2 mg/kg (i.v.) and 100 mg/kg (i.p)) exhibits low systematic plasma clearance (CL = 7 mL/min/kg) with terminal elimination half-life (T_{1/2}) of 2.22 h following a single i.v. administration. The normal liver blood flow in mice is 90 mL/min/kg and the V_{ss} (volume of distribution) is ~4-fold. Plasma concentrations is quantifiable up to 24 h with T_{max} of 0.50 h after i.p. administration^[1].

References:

[1]. Astudillo L et al. The Small Molecule IMR-1 Inhibits the Notch Transcriptional Activation Complex to Suppress Tumorigenesis. Cancer Res. 2016 Jun 15;76(12):3593-603.

CAIndexNames:

Acetic acid, 2-[2-methoxy-4-[(4-oxo-2-thioxo-5-thiazolidinylidene)methyl]phenoxy]-

SMILES:

O=C(O)COC1=CC=C(/C=C(SC(N2)=S)\C2=O)C=C1OC

Caution: Product has not been fully validated for medical applications. For research use only.

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