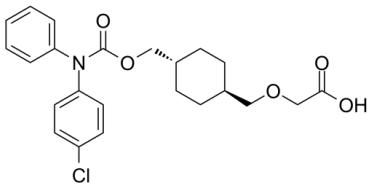
Data Sheet

Product Name:	Ralinepag
Cat. No.:	CS-0012350
CAS No.:	1187856-49-0
Molecular Formula:	C23H26ClNO5
Molecular Weight:	431.91
Target:	Prostaglandin Receptor
Pathway:	GPCR/G Protein
Solubility:	DMSO : 125 mg/mL (289.41 mM; Need ultrasonic and warming)



BIOLOGICAL ACTIVITY:

Ralinepag is a potent, orally bioavailable and non-prostanoid **prostacyclin (IP) receptor** agonist, with **EC_{50}**s of 8.5 nM, 530 nM and 850 nM for human and rat IP receptor and human DP1 receptor, respectively. IC50 & Target: EC50: 8.5 nM (Human IP receptor), 530 nM (Rat IP receptor), 850 nM (Human DP1 receptor)[1] **In Vitro:** Ralinepag is a potent non-prostanoid prostacyclin receptor agonist, with EC_{50}s of 8.5 nM, 530 nM and 850 nM for human and rat IP receptor and human DP1 receptor, respectively. Ralinepag (5c) has potent receptor binding affinity at prostaglandin receptor, with K_is of 1.2 nM, 3 nM, 76 nM, and 256 nM for monkey, human, rat, and dog IP receptor (ligand, [^{3}H]-iloprost), and 2.6 μM, 9.6 μM, 610 nM, 143 nM, and 678 nM for human DP1, EP1, EP2, EP3v6 and EP4 receptors (ligand, [^{3}H]-PGE2), respectively. Moreover, Ralinepag shows no effect on cytochrome P450 enzymes (IC_{50} > 50 μM for CYPs 1A2, 2D6, 3A4 2C8, 2C9, and 2C19) or hERG channel functional activity in a patch clamp assay (IC_{50} > 30 μM). Ralinepag also inhibits the ADP-induced human platelet aggregation, with an IC_{50} of 38 nM[1]. **In Vivo:** Ralinepag (30 mg/kg, p.o.) markedly reduces the monocrotaline (MCT)-induced increase in pulmonary arterial pressure and pulmonary vessel wall thickness in rats[1].

References:

[1]. Tran TA, et al. Discovery of 2-(((1r,4r)-4-(((4-Chlorophenyl)(phenyl)carbamoyl)oxy)methyl)cyclohexyl)methoxy)acetate (Ralinepag): An Orally Active Prostacyclin Receptor Agonist for the Treatment of Pulmonary Arterial Hypertension. J Med Chem. 2017 Feb 9;60(3):913-927.

CAIndexNames:

Acetic acid, 2-[[trans-4-[[[[(4-chlorophenyl)phenylamino]carbonyl]oxy]methyl]cyclohexyl]methoxy]-

SMILES:

O=C(O)COC[C@H]1CC[C@H](COC(N(C2=CC=C(Cl)C=C2)C3=CC=CC=C3)=O)CC1

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

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