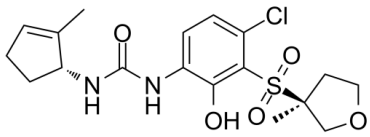
Data Sheet

Product Name:	CXCR2-IN-2
Cat. No.:	CS-0079459
CAS No.:	1838123-21-9
Molecular Formula:	$C_{18}H_{23}ClN_2O_5S$
Molecular Weight:	414.90
Target:	CXCR
Pathway:	GPCR/G Protein; Immunology/Inflammation
Solubility:	DMSO : 240 mg/mL (578.45 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

CXCR2-IN-2 is a selective, brain penetrant, and orally bioavailable **CXCR2** antagonist (**IC_{50}**=5.2 nM/1 nM in β-arrestin assay/CXCR2 Tango assay, respectively). CXCR2-IN-2 displays ~730-fold selectivity over CXCR1 and >1900-fold selectivity over all other chemokine receptors. CXCR2-IN-2 inhibits human whole blood Gro-α induced CD11b expression with an IC_{50} of 0.04 μM[1]. **In Vivo:** CXCR2-IN-2 (compound 68) (1-10 mg/kg; p.o.; twice daily for 3 days) dose-dependently reduces neutrophil infiltration in vivo in rat and mouse air pouch models[1].

References:

[1]. Lu H, et al. Discovery of Novel 1-Cyclopentenyl-3-phenylureas as Selective, Brain Penetrant, and Orally Bioavailable CXCR2 Antagonists. J Med Chem. 2018;61(6):2518-2532.

CAIndexNames:

Urea, N-[4-chloro-2-hydroxy-3-[[(3S)-tetrahydro-3-methyl-3-furanyl]sulfonyl]phenyl]-N'-[(1R)-2-methyl-2-cyclopenten-1-yl]-

SMILES:

O=C(N[C@H]1C(C)=CCC1)NC2=CC=C(Cl)C(S(=O)([C@]3(C)COCC3)=O)=C2O

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

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