



Data Sheet

 Product Name:
 CXCR2-IN-1

 Cat. No.:
 CS-6467

 CAS No.:
 1873376-49-8

Molecular Formula: C19H20Cl2FN3O4S

Molecular Weight: 476.35 Target: CXCR

Pathway: GPCR/G Protein; Immunology/Inflammation

Solubility: DMSO: 5.4 mg/mL (11.34 mM; Need ultrasonic and warming)

BIOLOGICAL ACTIVITY:

CXCR2-IN-1 is a central nervous system penetrant CXCR2 antagonists with a pIC₅₀ of 9.3. IC50 & Target: pIC50: 9.3 (CXCR2)^[1] In Vitro: CXCR2 plays an important role in the activation and recruitment of neutrophils to sites of inflammation. CXCR2-IN-1 shows favorable central nervous system penetration property (Br/Bl>0.45)^[1]. In Vivo: CXCR2-IN-1 shows efficacy in a cuprizone-induced demyelination model through oral administration, providing evidence to support CXCR2 to be a potential therapeutic target to treat demyelinating diseases such as multiple sclerosis^[1].

PROTOCOL (Extracted from published papers and Only for reference)

Animal Administration: ^[1]Mouse: Mice are fed with cuprizone for 5 weeks to cause demyelinating lesions in the CNS and then orally administrated with CXCR2-IN-1 for 9 consecutive days at doses of 30 and 100 mg/kg twice daily^[1].

References:

[1]. Xu H, et al. Discovery of CNS Penetrant CXCR2 Antagonists for the Potential Treatment of CNS Demyelinating Disorders. ACS Med Chem Lett. 2016 Feb 8;7(4):397-402.

CAIndexNames:

Urea, N-(2-chloro-3-fluorophenyl)-N'-[4-chloro-2-hydroxy-3-[(1-methyl-4-piperidinyl)sulfonyl]phenyl]-

SMILES:

 $\mathsf{CIC1} = \mathsf{CC} = \mathsf{C}(\mathsf{NC}(\mathsf{NC2} = \mathsf{CC} = \mathsf{CC}(\mathsf{F}) = \mathsf{C2CI}) = \mathsf{O})\mathsf{C}(\mathsf{O}) = \mathsf{C1S}(=\mathsf{O})(\mathsf{C3CCN}(\mathsf{C})\mathsf{CC3}) = \mathsf{O}$

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

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