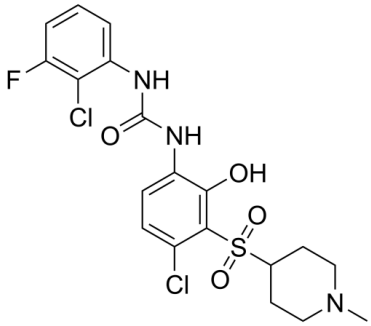
Data Sheet

Product Name:	CXCR2-IN-1
Cat. No.:	CS-6467
CAS No.:	1873376-49-8
Molecular Formula:	$C_{19}H_{20}Cl_2FN_3O_4S$
Molecular Weight:	476.35
Target:	CXCR
Pathway:	GPCR/G Protein; Immunology/Inflammation
Solubility:	DMSO : 5.4 mg/mL (ultrasonic;warming)



BIOLOGICAL ACTIVITY:

CXCR2-IN-1 is a central nervous system penetrant **CXCR2** antagonist with a **pIC_{50}** 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 (compound 22) 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]Mice: 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:

ClC1=CC=C(NC(NC2=CC=CC(F)=C2Cl)=O)C(O)=C1S(=O)(C3CCN(C)CC3)=O

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