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DATASHEET

LUF7591 (Covalent CCR2 ligand Compound 14)

Product overview

Name	LUF7591 (Covalent CCR2 ligand Compound 14)
Cat No	HB7329
Biological description	Novel, chemokine CCR2 covalent negative allosteric modulator (NAM) (apparent pK_i values at CCR2 are 8.7 and 9.2 (after 4h), where a K_i shift indicates a covalent mode of action). Binds intracellularly and forms a covalent bond with one of three proximal cysteine residues of CCR2.
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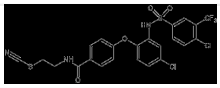
Biological action	NAM
Purity	>95%
Description	Novel, intracellular covalent chemokine CCR2 negative allosteric modulator (NAM). Binds irreversibly.

Solubility & Handling

Storage instructions	-20°C
Solubility overview	Soluble in DMSO
Important	This product is for RESEARCH USE ONLY and is not intended for therapeutic or diagnostic use. Not for human or veterinary use

Chemical Data

Chemical name	2-[[4-[4-Chloro-2-[[4-chloro-3-(trifluoromethyl)phenyl]sulfonylamino]phenoxy]benzoyl]amino]ethyl thiocyanate
Molecular Weight	590.4
Chemical structure	
Molecular Formula	$C_{23}H_{16}Cl_2F_3N_3O_4S_2$
PubChem identifier	162666730
SMILES	C1=CC(=CC=C1C(=O)NCCSC#N)OC2=C(C=C(C=C2)Cl)NS(=O)(=O)C3=CC(=C(C=C3)Cl)C(F)(F)F
InChiKey	FKIPEBVDUWFIIM-UHFFFAOYSA-N
Licensing details	Sold under license from the Oncode Cancer Institute and Universiteit Leiden

References

Design and Characterization of an Intracellular Covalent Ligand for CC Chemokine Receptor 2.

Ortiz Zacarías NV et al (2021) Journal of medicinal chemistry 64

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