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DATASHEET

LUF7746

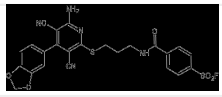
Product overview

Name	LUF7746
Cat No	HB6921
Biological description	The first covalent hA_1AR partial agonist which irreversibly activates the receptor (apparent pK_i values at CHO-hA_1ARs are 7.7 and 8.4 (after 4h), where a K_i shift indicates a covalent mode of action). Shown to covalently bind to the A_1AR receptor under many different experimental conditions. The $Y271^{7.36}$ tyrosine residue within the hA_1AR binding pocket has been demonstrated as the primary anchor point for this covalent interaction. LUF7746 is a valuable probe for further mapping the receptor activation process. *Sold under license from the Oncode Cancer Institute and Universiteit Leiden*
Biological action	Agonist
Purity	>95%
Description	The first covalent hA_1AR partial agonist. 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	4-((3-((6-Amino-4-(benzo[d][1,3]dioxol-5-yl)-3,5-dicyanopyridin-2-yl)thio)propyl)carbamoyl)benzenesulfonyl fluoride
Molecular Weight	539.6
Chemical structure	
Molecular Formula	$C_{24}H_{18}FN_5O_5S_2$
PubChem identifier	167312225
SMILES	C1OC2=C(O1)C=C(C=C2)C3=C(C(=NC(=C3C#N)SCCCNC(=O)C4=CC=C(C=C4)S(=O)(=O)F)N)C#N
InChiKey	ZDQUUOSIWXZJJE-UHFFFAOYSA-N
Licensing details	Sold under license from the Oncode Cancer Institute and Universiteit Leiden

References

Design and pharmacological profile of a novel covalent partial agonist for the adenosine A(1) receptor.

Yang X et al (2020) Biochemical pharmacology 180
PubMedID 32653590

Design and pharmacological profile of a novel covalent partial agonist for the adenosine A(1) receptor.

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A Chemical Biological Approach to Study G Protein-Coupled Receptors: Labeling the Adenosine A(1) Receptor Using an Electrophilic Covalent Probe.

Beerkens BLH et al (2022) ACS chemical biology 17

PubMedID 36279267