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DATASHEET

Iperoxo

Product overview

Name	Iperoxo
Cat No	HB9785
Biological action	Agonist
Description	Potent muscarinic acetylcholine receptor superagonist. Also binds the hM3R-miniG_q DREADD receptor.

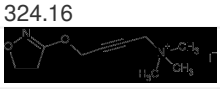
Biological Data

Biological description	Potent muscarinic acetylcholine receptor (mAChR) superagonist (EC_{50} = 2.12 and 8.47 at M2 and M4 respectively). Used to solve the WT-hM3R structure. Recently used to report the cryogenic electron microscopy high-resolution structure of the hM3R-miniG_q DREADD receptor complex to provide an insight into the agonist selectivity of DREADDs. This may assist structure-guided discovery of further chemogenetic tools.

Solubility & Handling

Storage instructions	-20°C
Solubility overview	Soluble in water (50 mM), and in DMSO (100 mM)
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-[(4,5-dihydro-1,2-oxazol-3-yl)oxy]-N,N,N-trimethylbut-2-yn-1-aminium iodide
Molecular Weight	324.16
Chemical structure	
Molecular Formula	$C_{10}H_{17}IN_2O_2$
SMILES	[I-].C[N+](C)(C)CC#CCOC=1CCON=1
Source	Synthetic
InChi	InChI=1S/C10H17N2O2.HI/c1-12(2,3)7-4-5-8-13-10-6-9-14-11-10;/h6-9H2,1-3H3;1H/q+1;/p-1
InChiKey	XWEOIAMCTHLJJB-UHFFFAOYSA-M

References

Molecular basis for selective activation of DREADD-based chemogenetics.

Zhang S et al (2022) Nature 612
PubMedID 36450989

Agonists with supraphysiological efficacy at the muscarinic M2 ACh receptor.

Schrage R et al (2013) British journal of pharmacology 169
PubMedID 23062057

New insight into active muscarinic receptors with the novel radioagonist [^{3}H]iperoxo.

Schrage R et al (2014) Biochemical pharmacology 90

PubMedID 24863257