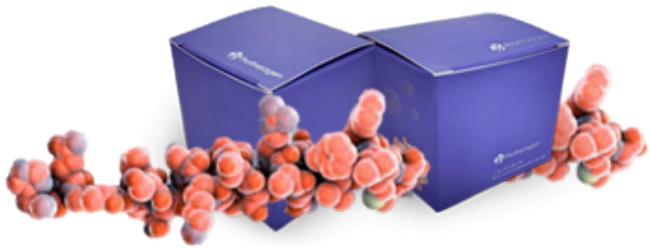
Protheragen
Obesity



LY2409881

Cat. No.:	OB0225WX-2701
Appearance:	Solid
Purity:	≥99%
Identity:	Confirmed by NMR, and HPLC.
Size:	5 mg; 25 mg; 100 mg

This product is for research use only and is not intended for diagnostic use.

Product Overview

Description	LY2409881 acts as a high-potency IKK2 inhibitor with an IC50 of 30 nM, demonstra ting more than 10-fold selectivity compared to IKK1 and other standard kinases.
Synonym	946518-60-1; LY2409881 trihydrochloride; LY2409881 (trihydrochloride); 2-(5-chlo ro-2-((3-(4-methylpiperazin-1-yl)propyl)amino)pyrimidin-4-yl)-*N*-cycloprop ylbenzo[b]thiophene-4-carboxamide trihydrochloride; s7697; 2-(5-chloro-2-(3-(4-m ethylpiperazin-1-yl)propylamino)pyrimidin-4-yl)-*N*-cyclopropylbenzo[b]thio phene-4-carboxamide trihydrochloride; 2-{5-chloro-2-[3-(4-methylpiperazin-1-yl)- propylamino]-pyrimidin-4-yl}-benzo[b]thiophene-4-carboxylic acid cyclopropylamid e tri-hydrochloride; LY-2409881 trihydrochloride; LY2409881 3HCl; 2-(5-chloro-2- {[3-(4-methylpiperazin-1-yl)propyl]amino}pyrimidin-4-yl)-*N*-cyclopropyl-1- benzothiophene-4-carboxamide trihydrochloride
CAS No.	946518-60-1
Compound CID	68856073
Formula	$C_{24}H_{32}Cl_4N_6OS$
Formula Weight	594.43

Specification

IUPAC Name	2-[5-Chloro-2-[3-(4-methylpiperazin-1-yl)propylamino]pyrimidin-4-yl]-*N*-cy clopropyl-1-benzothiophene-4-carboxamide;trihydrochloride

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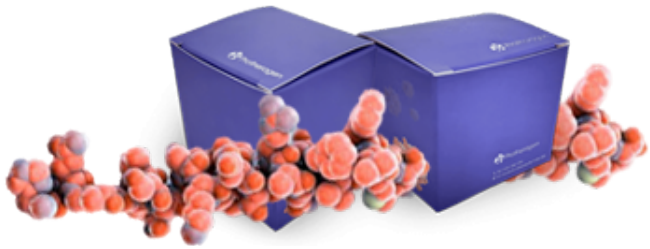

InChI	InChI=1S/C24H29ClN6OS.3ClH/c1-30-10-12-31(13-11-30)9-3-8-26-24-27-15-19(25)22(29-24)21-14-18-17(4-2-5-20(18)33-21)23(32)28-16-6-7-16;;;/h2,4-5,14-16H,3,6-13H2,1H3,(H,28,32)(H,26,27,29);3*1H
InChI Key	IEXCRLAGBWKVPW-UHFFFAOYSA-N
SMILES string	CN1CCN(CC1)CCCNC2=NC=C(C(=N2)C3=CC4=C(C=CC=C4S3)C(=O)NC5CC5)Cl.Cl.Cl.Cl
Stability	3 years in powder form.
Storage	Storage at -20°C.
Applications	LY2409881 is utilized in oncology research as a selective inhibitor of IKK-epsil on to investigate the disruption of oncogenic signaling and the sensitization of malignant cells to therapeutic agents.

Library Information

Target	IκB/IKK
Receptor	IKK2
Pathways	NF-κB
Plate Number	L6700-09
Empty Location	a1-h1; a12-h12
Container	96-well plate
Formulation	10mM DMSO
DMSO Max Solubility	20 mg/mL; 33.65 mM
ALogP	5.147
HBA_Count	3
HBD_Count	2
Rotatable Bond	8

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