Product Data Sheet

Product Name: GNE-616
Cat. No.: GC36169

Chemical Properties

Cas. No.	2349371-81-7		
SMILES	O=S(C1=C(F)C=C2[C@@H](N3[C@@H](C4=NC=CC=C4)C[C@@H](C(F)(F)F)CC3)CCOC2=C1)(NC5=NC=NC=C5)=O		
Formula	$C_{24}H_{23}F_4N_5O_3S$	M.Wt	537.53
Solubility	Soluble in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	GNE-616		

Background

GNE-616 is a highly potent, metabolically stable, orally bioavailable, and subtype selective Nav1.7 inhibitor (Ki of 0.79 nM and Kd of 0.38 nM for hNav1.7) for the treatment of chronic pain. GNE-616 shows >1000 nM Kd and >2500-fold selectivity over hNav1.1, hNav1.3, hNav1.4, and hNav1.5. Selectivity over hNav1.2 and hNav1.6 is more modest at 31- and 73-fold, respectively[1]. Ki: 0.79 nM (hNav1.7)[1]Kd: 0.38 nM (hNav1.7), 12 nM (hNav1.2), 29 nM (hNav1.6)[1]

Site-directed mutagenesis is critical for the isoform selectivity profile of GNE-616 (hNav1.7, Kd: Y1537s/W1538=170±67 nM, V1541=3.9±1.1 nM, Y1537s/W1538/V1541=790±350 nM)[1].

GNE-616 shows robust activity in a Nav1.7-dependent inherited erythromelalgia (IEM) PK/PD model with an EC50 of 740 nM and EC50,u of 9.6 nM[1].

[1]. McKerrall SJ, et al. Structure- and Ligand-Based Discovery of Chromane Arylsulfonamide Nav1.7 Inhibitors for the Treatment of Chronic Pain. J Med Chem. 2019

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com
Address: 10292 Central Ave. #205, Montclair, CA, USA

Apr 25;62(8):4091-4109.

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com
Address: 10292 Central Ave. #205, Montclair, CA, USA