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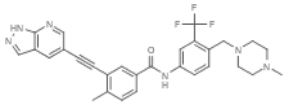
Datasheet (Version 1.0)

Product Name	:	GZD 824
Synonyms	:	GZD824; GZD 824; GZD-824
Cat No.	:	M17912
CAS Number	:	1257628-77-5
Molecular Formula	:	C29H27F3N6O
Formula Weight	:	532.57
Chemical Name	:	3-((1H-pyrazolo[3,4-b]pyridin-5-yl)ethynyl)-4-methyl-N-(4-((4-methylpiperazin-1-yl)methyl)-3-(trifluoromethyl)phenyl)benzamide
Description	:	GZD824 is a novel orally bioavailable inhibitor against a broad spectrum of Bcr-Abl mutants including T315I. GZD824 tightly bound to Bcr-Abl(WT) and Bcr-Abl(T315I) with K(d) values of 0.32 and 0.71 nM, respectively, and strongly inhibited the kinase functions with nanomolar IC(50) values. GZD824 potently suppressed proliferation of Bcr-Abl-positive K562 and Ku812 human CML cells with IC(50) values of 0.2 and 0.13 nM, respectively. GZD824 also displayed good oral bioavailability (48.7%), a reasonable half-life (10.6 h), and promising in vivo antitumor efficacy. It induced tumor regression in mouse xenograft tumor models driven by Bcr-Abl(WT) or the mutants and significantly improved the survival of mice bearing an allograft leukemia model with Ba/F3 cells harboring Bcr-Abl(T315I). GZD824 represents a promising lead candidate for development of Bcr-Abl inhibitors to overcome acquired imatinib resistance.
Pathway	:	Endocrinology/Hormones
Target	:	AChR
Receptor	:	Abl (E254K)
Solubility	:	DMSO : ≥ 100 mg/mL; 187.77 mM
SMILES	:	CN1CCN(Cc2c(cc(NC(=O)c3cc(C#Cc4cc5c([nH]nc5)nc4)c(C)cc3)cc2)C(F)(F)F)CC1
Storage	:	(-20℃)
Stability	:	≥ 2 years
Reference	:	



1. Ren X, et al. J Med Chem. 2013, 56(3), 879-894.