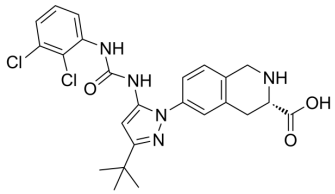
BCR-ABL-IN-2

Cat. No.:	HY-18819
CAS No.:	897369-18-5
Molecular Formula:	$C_{24}H_{25}Cl_2N_5O_3$
Molecular Weight:	502.39
Target:	Bcr-Abl
Pathway:	Protein Tyrosine Kinase/RTK
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	BCR-ABL-IN-2 is an inhibitor of BCR-ABL1 tyrosine kinase, with IC_{50}s of 57 nM, 773 nm for $ABL1^{native}$ and $ABL1^{T315I}$, respectively.
IC_{50} & Target	IC50: 57 nM ($ABL1^{native}$), 773 nM ($ABL1^{T315I}$)[1].
In Vitro	BCR-ABL-IN-2 (Compound 1) contains a urea moiety to allow a hydrogen bond with the conserved K271-E286 salt bridge of ABL1, a t-butyl moiety to bind into the hydrophobic spine at the third pocket position, and a 2,3-dichlorophenyl ring to stabilize the DFG-phenylalanine F382 in the Type II-out conformation. BCR-ABL-IN-2 exhibits an IC_{50} of 57 nM for $ABL1^{native}$ and an IC_{50} of 773 nM for $ABL1^{T315I}$[1]. Despite ABL, BCR-ABL-IN-2 can also inhibit KDR, BRaf, p38 kinase with IC_{50}s of 1.8 μM, 0.23 μM, 6.3 nM, 43 nM, respectively[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Chan WW, et al. Conformational control inhibition of the BCR-ABL1 tyrosine kinase, including the gatekeeper T315I mutant, by the switch-control inhibitor DCC-2036. Cancer Cell. 2011 Apr 12;19(4):556-68.

[2]. ARYL SULFONOHYDRAZIDES. US 2008/0113967 A1.

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