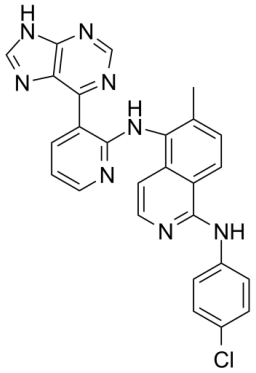
Data Sheet

Product Name:	B-Raf inhibitor 1
Cat. No.:	CS-2182
CAS No.:	1093100-40-3
Molecular Formula:	C26H19ClN8
Molecular Weight:	478.94
Target:	Raf
Pathway:	MAPK/ERK Pathway
Solubility:	DMSO : ≥ 53 mg/mL (110.66 mM)



BIOLOGICAL ACTIVITY:

B-Raf inhibitor 1 is a potent **Raf** kinase inhibitor with **K**$_i$s of 1 nM, 1 nM, and 0.3 nM for B-Raf^{WT}, B-Raf^{V600E}, and C-Raf, respectively. IC50 & Target: Ki: 1 nM (B-Raf^{WT}), 1 nM (B-Raf^{V600E}), 0.3 nM (C-Raf)[1] **In Vitro:** B-Raf inhibitor 1 (Compound 13) inhibits A375 and HCT-116 proliferation with IC_{50}s of 0.31 and 0.72 μM, respectively. B-Raf inhibitor 1 (Compound 13) binds to and stabilizes B-Raf in a DFG-out, inactive conformation in which the ATP pocket is partially filled by Phe595 and Gly596 from the DFG motif. B-Raf inhibitor 1 (Compound 13) additionally exhibits low micromolar inhibition against wild type B-Raf cell lines, which may be due to off-target kinase activities or alternatively to pan-Raf inhibition, including Raf dimers[1].

References:

[1]. Wang X, et al. Conformation-specific effects of Raf kinase inhibitors. J Med Chem. 2012 Sep 13;55(17):7332-41.

CAIndexNames:

1,5-Isoquinolinediamine, N1-(4-chlorophenyl)-6-methyl-N5-[3-(9H-purin-6-yl)-2-pyridinyl]-

SMILES:

CC1=CC=C2C(C=CN=C2NC3=CC=C(Cl)C=C3)=C1NC4=NC=CC=C4C5=NC=NC6=C5N=CN6

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