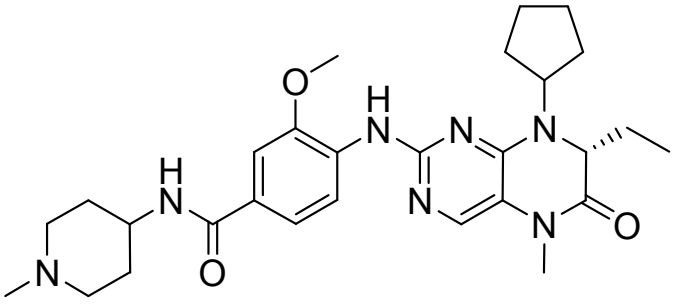
(R)-BI-2536

SYN-1019



4-((R)-8-cyclopentyl-7-ethyl-5,6,7,8-tetrahydro-5-methyl-6-oxopteridin-2-ylamino)-3-methoxy-N-(1-methylpiperidin-4-yl)benzamide

CAS Registry No.: 755038-02-9

Smiles String:
CC[C@@H]1C(=O)N(c2cnc(nc2N1C3CCCC3)Nc4ccc(cc4OC)C(=O)NC5CCN(CC5)C)C

Molecular Weight: 521.65

Molecular Formula: C28H39N7O3

Lot Number: Refer to vial

1H-NMR: Available on request

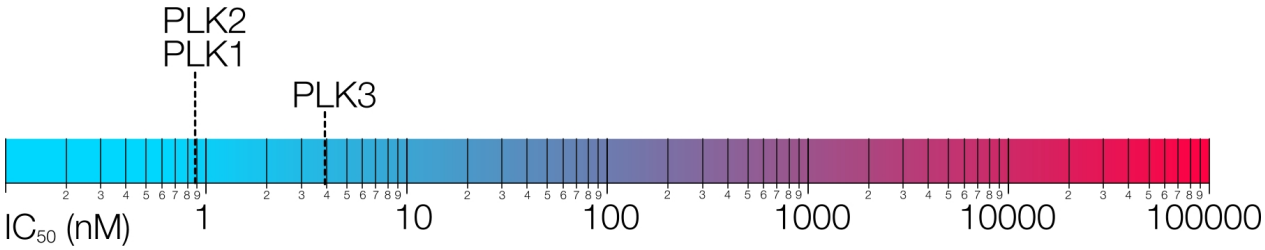
HPLC (Purity): > 95.0% @ 254 nm

ES-MS: Available on request

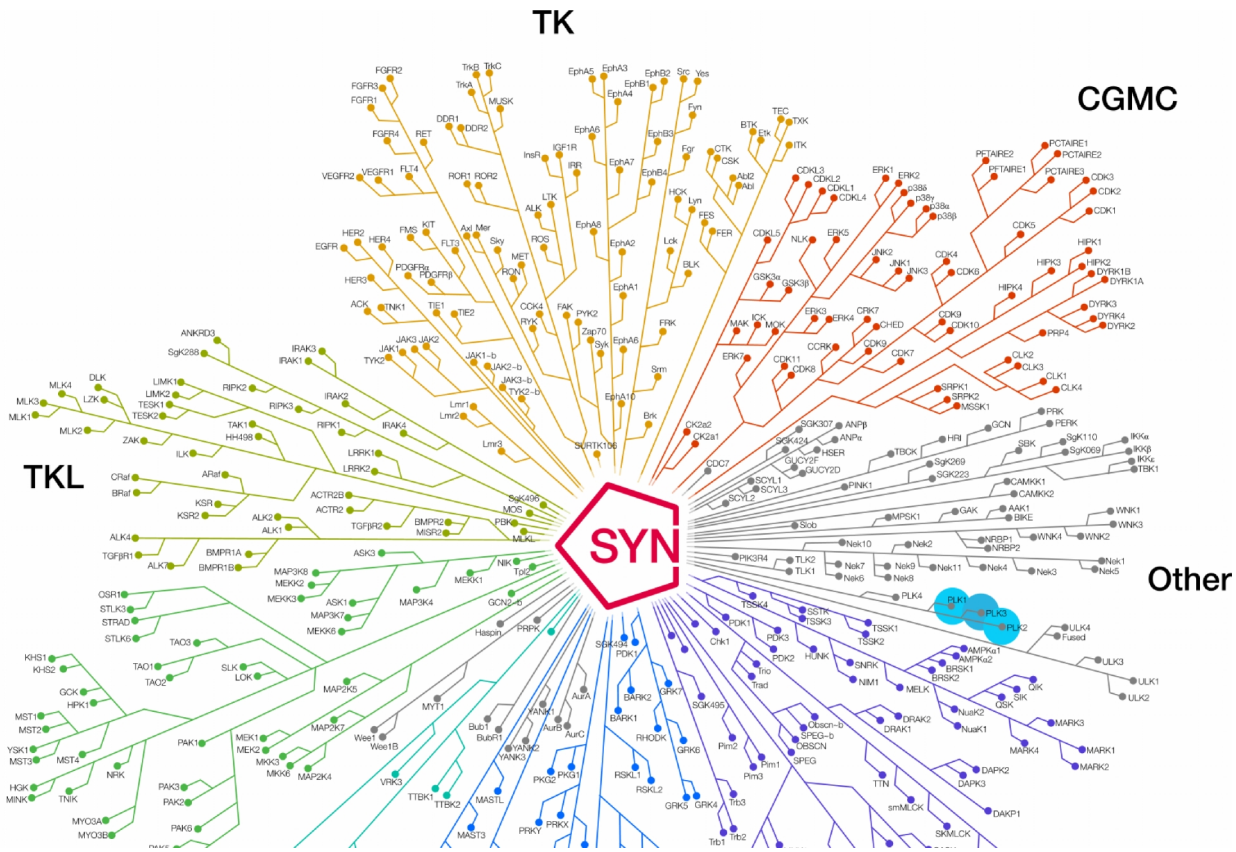
Description:

Polo-like kinase 1 (Plk1) is a regulator of the cell cycle that has been implicated in the pathology of many cancers. BI-2536 is a potent and selective small-molecule inhibitor of mammalian Plk1. It has inhibitory activity at subnanomolar concentrations and inhibits tumor growth in multiple tumor lines with IC50 values below 1 μM. BI-2536 also shows an >1,000-fold selectivity for PIK1 versus a large panel of other kinases. BI-2536 also demonstrated low Kd values against sister kinases PLK2 and PLK3. Preclinical studies in human cancer cell lines have shown that BI 2536 disrupts spindle assembly, resulting in mitotic arrest and inducing apoptosis. BI-2536 is currently in clinical trials against several types of solid tumor cancers.

Biological Activity



Kinome Mapping



Shipping and Storage Temperature

Shipping:
Ambient

Storage:
2 years -20C, Powder 1 month, -4C in DMSO, More than one month -80C in DMSO

Solubility

DMSO 21mg/mL, Ethanol 100mg/mL

Preparing Stock Solutions

Stock Solution (1ml DMSO)	1mM	10mM	20mM	50mM
Mass(mg)	0.5217	5.2170	10.4340	26.0850

References

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2. Wang HY, Cao ZX, Li LL, Jiang PD, Zhao YL, Luo SD, Yang L, Wei YQ, Yang SY . Pharmacophore modeling and virtual screening for designing potential PLK1 inhibitors. Bioorg Med Chem Lett. 2008 Sep 15;18(18):4972-7. doi: 10.1016/j.bmcl.2008.08.033. Epub 2008 Aug 14.

3. Zhang Q, Xia Z, Mitten MJ, Lasko LM, Klinghofer V, Bouska J, Johnson EF, Penning TD, Luo Y, Giranda VL, Shoemaker AR, Stewart KD, Djuric SW, Vasudevan A . Hit to Lead optimization of a novel class of squarate-containing polo-like kinases inhibitors. Bioorg Med Chem Lett. 2012 Dec 15;22(24):7615-22. doi: 10.1016/j.bmcl.2012.10.009. Epub 2012 Oct 11.

Ordering Information

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