

LEE011

SYN-1213

7-cyclopentyl-N,N-dimethyl-2-[(5-piperazin-1-yl)pyridin-2-yl]amino]pyrrolo[2,3-d]pyrimidine-6-carboxamide

CAS Registry No.: 1211441-98-3

Smiles String:

CN(C)C(=O)C1=CC2=CN=C(N=C2N1C3CCC3)NC4=NC=C(C=C4)N5CCNCC5

Molecular Weight: 434.54

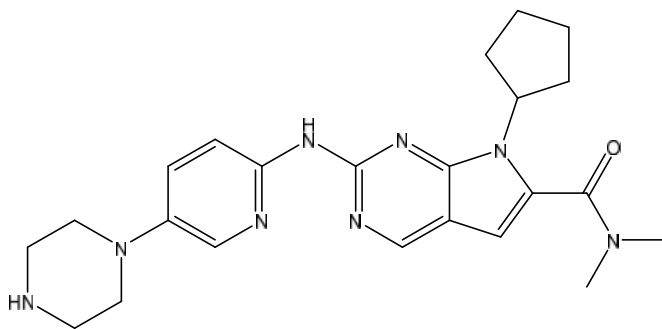
Molecular Formula: C₂₃H₃₀N₈O

Lot Number: Refer to vial

¹H-NMR: Available on request

HPLC (Purity): > 95.0% @ 254 nm

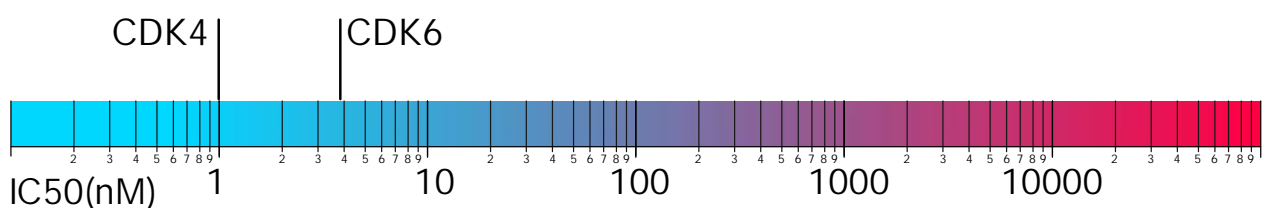
ES-MS: Available on request



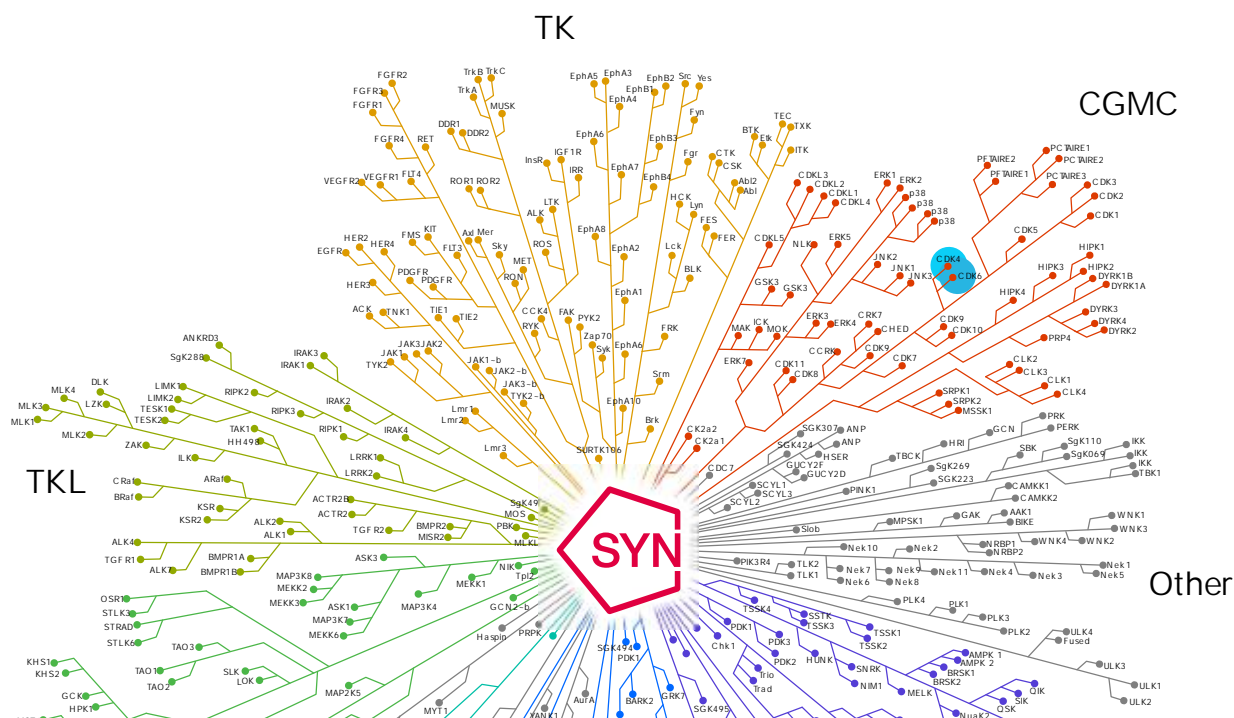
Description:

LEE011 is an orally available cyclin-dependent kinase (CDK) inhibitor targeting cyclin D1/CDK4 and cyclin D3/CDK6 cell cycle pathway, with potential antineoplastic activity. It specifically inhibits CDK4 and 6, thereby inhibiting retinoblastoma (Rb) protein phosphorylation. Inhibition of Rb phosphorylation prevents CDK-mediated G1-S phase transition, thereby arresting the cell cycle in the G1 phase, suppressing DNA synthesis and inhibiting cancer cell growth. Overexpression of CDK4/6, as seen in certain types of cancer, causes cell cycle deregulation.

Biological Activity



Kinome Mapping



Shipping and Storage Temperature

Shipping:
Ambient

Storage:
3 Months at -4C, >2 Years at -20C

Solubility

DMSO 7mg/mL

Preparing Stock Solutions

Stock Solution (1ml DMSO)	1mM	10mM	20mM	50mM
Mass(mg)	0.434	4.345	8.690	21.727

References

1. Rader J, Russell MR, Hart LS, Nakazawa MS, Belcastro LT, Martinez D, Li Y, Carpenter EL, Attiyeh EF, Diskin SJ, Kim S, Parasuraman S, Caponigro G, Schnepf RW, Wood AC, Pawel B, Cole KA, Maris JM. Dual CDK4/CDK6 inhibition induces cell-cycle arrest and senescence in neuroblastoma. *Clin Cancer Res*. 2013 Nov 15;19(22):6173-82. doi: 10.1158/1078-0432.CCR-13-1675. Epub 2013 Sep 17. PubMed PMID: 24045179; PubMed Central PMCID: PMC3844928.
2. <https://www.google.com/patents/WO2010020675A1?cl=en>
3. Sunkyu Kim, Alice Loo, Rajiv Chopra, Giordano Caponigro, Alan Huang, Sadhna Vora, Sudha Parasuraman, Steve Howard, Nicholas Keen, William Sellers, Christopher Brain. LEE011: An orally bioavailable, selective small molecule inhibitor of CDK4/6– Reactivating Rb in cancer. [abstract]. In: Proceedings of the AACR-NCI-EORTC International Conference: Molecular Targets and Cancer Therapeutics; 2013 Oct 19-23; Boston, MA. Philadelphia (PA): AACR; *Mol Cancer Ther* 2013;12(11 Suppl):Abstract nr PR02.
4. <http://www.fda.gov/downloads/AdvisoryCommittees/CommitteesMeetingMaterials/Drugs/OncologicDrugsAdvisoryCommittee/UCM375648.pdf>
5. <http://pubchem.ncbi.nlm.nih.gov//compound/44631912>

Ordering Information

To order more of this or any other SYNkinase compound, go to synkinase.com, Call us Toll Free (US Only) at 1- 877-854-6273 or email orders@synkinase.com.

Product Datasheet (Rev. 1.1)