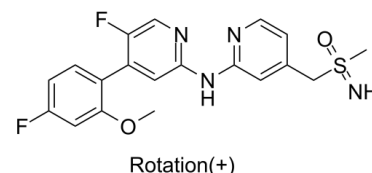


Data Sheet

Product Name:	(+)-Enitociclib
Cat. No.:	CS-0023124
CAS No.:	1610358-56-9
Molecular Formula:	C ₁₉ H ₁₈ F ₂ N ₄ O ₂ S
Molecular Weight:	404.43
Target:	CDK
Pathway:	Cell Cycle/DNA Damage
Solubility:	DMSO : 113.3 mg/mL (280.15 mM; Need ultrasonic and warming)



BIOLOGICAL ACTIVITY:

(+)-Enitociclib ((+)-BAY-1251152) is an enantiomer of BAY-1251152 with rotation (+). (+)-Enitociclib is a potent and selective **CDK9** inhibitor with an **IC₅₀** of 3 nM. (+)-Enitociclib has anti-tumour activity^{[1][2]}. **In Vitro:** (+)-Enitociclib (Example 2) inhibits HeLa, HeLa-MaTu-ADR, NCI-H460, DU145, Caco-2, B16F10, A2780 and MOLM-13 cells proliferation with IC₅₀ values of 110 nM, 33 nM, 75 nM, 33 nM, 62 nM, 240 nM, 110 nM and 29 nM, respectively^[1].

An efficient inhibition of the proliferation of both ABC (Activated B-cell type) and GCB (Germinal-centre B-cell type) subtypes of diffuse large B-cell lymphoma (DLBCL) by (+)-Enitociclib (Compound A')^[2]. **In Vivo:** (+)-Enitociclib (Compound A'; 10 mg/kg; intravenous injection; once every seven days; for 14 days; female SCID mice) treatment reaches a Treatment to Control ratios (T/C) by area of 0.29 and a T/C by weight of 0.24. (+)-Enitociclib inhibits tumour growth and had good tolerability^[2].

References:

[1]. Ulrich LÜCKING, et al. 5-fluoro-n-(pyridin-2-yl)pyridin-2-amine derivatives containing a sulfoximine group. WO2014076091A1.

[2]. Use of Arne Scholz, et al. 5-fluoro-4-(4-fluoro-2-methoxyphenyl)-n-<4-[(s-methylsulfonylmethyl)]pyridin-2-yl>pyridin-2-amine for treating diffuse large b-cell lymphoma. WO2019158517A1.

CAIndexNames:

2-Pyridinamine, 5-fluoro-4-(4-fluoro-2-methoxyphenyl)-N-[4-[(S-methylsulfonylmethyl)]-2-pyridinyl]-, (+)-

SMILES:

N=S(CC1=CC(NC2=NC=C(F)C(C3=CC=C(F)C=C3OC)=C2)=NC=C1)(C)=O.[Rotation(+)]

Caution: Product has not been fully validated for medical applications. For research use only.

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