

Product Name	: Methylstat
Synonyms	: Methylstat
Cat No.	: M19349
CAS Number	: 1310877-95-2
Molecular Formula	: C ₂₈ H ₃₁ N ₃ O ₆
Formula Weight	: 505.56
Chemical Name	: (2E)-4-[Hydroxy[4-[[[4-[[[(1-naphthalenylamino)carbonyl]oxy)methyl]phenyl]methyl]-amino]butyl]amino]-4-oxo-2-buten-1-yl methyl ester
Description	Methylstat is a methyl ester prodrug of a Jumonji C domain-containing histone demethylase (JMJD) inhibitor that has favorable cell permeability. The free acid of methylstat inhibits JMJD2A, JMJD2C, JMJD2E, PHF8, and JMJD3 with IC₅₀ values of approximately 4.3, 3.4, 5.9, 10, and 43 μM, respectively, in an in vitro assay. Methylstat inhibits growth of the JMJD2C-sensitive esophageal cancer cell line KYSE150 with a GI₅₀ of 5.1 μM, whereas the free acid of methylstat did not inhibit cell growth up to 100 μM. Methylstat induces histone hypermethylation at multiple sites in a concentration-dependent manner (EC₅₀ for H3K4me3 and H3K9me3 = 10.3 and 8.6 μM in KYSE150 cells and 6.7 and 6.3 μM in MCF-7 cells, respectively).
Pathway	: Others
Target	: Other Targets
Receptor	: JMJD2A; JMJD2C; JMJD2E; PHF8; JMJD3
Solubility	: —
SMILES	: <chem>CCOC(=O)/C=C/C(N(O)CCCCNCC1=CC=C(COC(NC2=C3C=CC=CC3=CC=C2)=O)C=C1)=O</chem>
Storage	: (-20°C)
Stability	: ≥ 2 years
Reference	:

1. Luo, X., et al. Journal of the American Chemical Society 133(24), 9451-9456 (2011).

