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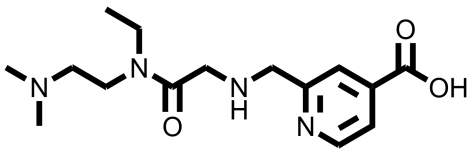
JARID1 Histone Demethylases Inhibitor – KDM5-C49

Chemical Name: 2-(((2-((2-(dimethylamino)ethyl)(ethyl)amino)-2-oxoethyl)amino)methyl)isonicotinic acid



Molecular Weight:	308.38
Formula:	$C_{15}H_{24}N_4O_3$
Purity:	≥98%
CAS#:	n/a
Solubility:	DMSO up to 100 mM
Storage	Powder: 4 °C 1 year DMSO: 4 °C 3 months -20 °C 1 year

Biological Activity:

KDM5-C49 is a potent and selective inhibitor of Jumonji AT-Rich Interactive Domain 1 (JARID1) histone demethylases. It has IC_{50} ~40 nM, 160 nM and 100 nM for KDM5A, KDM5B and KDM5C respectively. It has >100-fold selectivity over KDM4 and KDM6 etc. KDM5-C49 occupies the aKG-binding site. The highly polar carboxylate group of KDM5-C49 restricts its cellular permeability, so it has IC_{50} >1 μM for inhibiting demthylation of H3K4 in U2OS human osteosarcoma cell line and in human breast adenocarcinoma MCF7 tumor cell proliferation assay. Therefore KDM5-C70 was developed as a pro-drug, masking the polarity of the acid group of the KDM5-C49, for cellular assays and in vivo use.

How to Use:

In vitro: KDM5-C49 was used at 1-10 μM in vitro.

In vivo: n/a

Reference:

1. Marc Labelle, et al. Inhibitors of Histone Demethylases. (2014). PCT WO 2014053491
2. Johansson C, et al. Structural analysis of human KDM5B guides histone demethylase inhibitor development. (2016) Nat Chem Biol. 12(7):539-45.
3. Horton JR, et al. Structural Basis for KDM5A Histone Lysine Demethylase Inhibition by Diverse Compounds. (2016) Cell Chem Biol. 23(7):769-81.