

Product Data Sheet

Product Name: XY1
Cat. No.: GC19388

Chemical Properties

Cas. No. 1624117-53-8

SMILES O=C(NCC(N1CCCC1)=O)NC2=CC=C3C=CC=CC3=C2

Formula $C_{17}H_{19}N_3O_2$ M.Wt 297.35

Solubility DMSO : 67.5 mg/mL (227.01 mM) Storage Store at -20°C

General tips For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.

Structure



Background

XY1 is a very close analogue of SGC707 (a potent, selective, and non-competitive inhibitor of PRMT3 with IC₅₀ of 31 nM), but XY1 is completely inactive. Target: PRMT3. XY1 is a close analogue of SGC707, is completely inactive against PRMT3 at concentrations as high as 100 µM. XY1 contains a naphthyl group replacing the isoquinoline group, lacks the key hydrogen bond with T466. The naphthyl ring of XY1 could act as a weak hydrogen-bond acceptor, but this should come with a substantial enthalpic penalty. The more than 1000-fold potency loss of XY1 compared with SGC707 supports this analysis. It is unclear whether other factors such as electronic effects also contributed to

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the potency loss of XY1 compared with SGC707. SGC707 and XY1 are a pair of excellent tools for the biomedical community to further elucidate biological functions and disease associations of PRMT3.

References:

[1]. Kaniskan H, et al. A potent, selective and cell-active allosteric inhibitor of protein arginine methyltransferase 3 (PRMT3). *Angew Chem Int Ed Engl.* 2015 Apr 20;54(17):5166-70.

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