

# PRODUCT INFORMATION

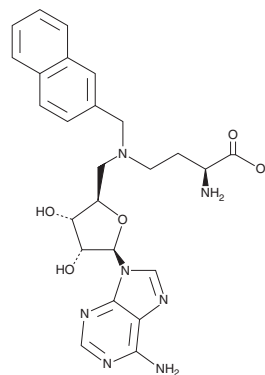


## Bisubstrate Inhibitor 78

Item No. 28567

**CAS Registry No.:** 2368247-39-4  
**Formal Name:** (S)-2-amino-4-(((2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl)methyl)(naphthalen-2-ylmethyl)amino)butanoic acid

**MF:** C<sub>25</sub>H<sub>29</sub>N<sub>7</sub>O<sub>5</sub>  
**FW:** 507.5  
**Purity:** ≥98%  
**UV/Vis.:** λ<sub>max</sub>: 224 nm  
**Supplied as:** A crystalline solid  
**Storage:** -20°C  
**Stability:** ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

### Laboratory Procedures

Bisubstrate inhibitor 78 is supplied as a crystalline solid. A stock solution may be made by dissolving the bisubstrate inhibitor 78 in the solvent of choice, which should be purged with an inert gas. Bisubstrate inhibitor 78 is slightly soluble in ethanol, methanol, DMSO, dimethyl formamide, and chloroform.

### Description

Bisubstrate inhibitor 78 is an inhibitor of nicotinamide N-methyltransferase (NNMT; IC<sub>50</sub> = 1.41 μM).<sup>1</sup> It binds the NNMT active site in the binding pockets for the NNMT substrates S-adenosyl-L-methionine (SAM) and nicotinamide (Item No. 11127). Bisubstrate inhibitor 78 is selective for NNMT over histone-lysine N-methyltransferase NSD2 and protein arginine methyltransferase 1 (PRMT1; IC<sub>50</sub>s = >50 μM for both). It reduces levels of 1-methylnicotinamide (MNA; Item No. 16604) in, and inhibits proliferation of, HSC-2 oral cancer cells when used at a concentration of 100 μM.

### Reference

1. Gao, Y., van Haren, M.J., Moret, E.E., *et al.* Bisubstrate inhibitors of nicotinamide N-methyltransferase (NNMT) with enhanced activity. *J. Med. Chem.* **62**(14), 6597-6614 (2019).

#### WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

#### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

#### WARRANTY AND LIMITATION OF REMEDY

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