

Catalog # 10-5733

M22

CAS# 864420-54-2

1-Benzyl-N-(2,4-dichlorophenethyl) piperidin-4-amine; or N-[2-(2,4-dichlorophenyl)ethyl]-1-(phenylmethyl)-4piperidinamine; NAE-IN-M22 Lot # S107101

Protein neddylation is a post-translational modification which transfers the ubiquitin-like protein NEDD8 to a lysine residue of the target substrate through a three-step enzymatic cascade and has been considered as a viable target for the development of new therapeutics for cancer. M22 is an inhibitor of NEDD8 activating enzyme (NAE) which was discovered by virtual screening of a small molecule library (50,000 compounds) against the active site of NAE.2 M22 is selective and reversible and inhibits NEDDylation of ubiquitinconjugating enzyme 12 (UBC12) in a cell-free assay employing recombinant human NAE. It selectively inhibits NEDDylation over SUMOylation and ubiquitination in A549 cells and inhibits their growth (GI₅₀ = 5.5 μM). It has been shown to inhibit tumor growth in a mouse xenograft model (at 60 mg/kg).²

- 1) Zhong et al. (2012), Discovery of a natural product inhibitor targeting protein neddylation by structure-based virtual screening; Biochimie, 94 2457
- 2) Lu et al. (2016), Discovery of a novel NEDD8 activating enzyme inhibitor with piperidin-4-amine scaffold by structure-based virtual screening; ACS Chem. Biol., 11 1901

PHYSICAL DATA

Molecular Weight: 363.33 Molecular Formula: $C_{20}H_{24}CI_2N_2$ Purity: >98% by TLC

NMR: (Conforms)

Solubility: DMSO (40 mg/ml) Physical Description: Off-white solid

Storage and Stability: Store as supplied desiccated at -20°C for up to 2 years from the date of purchase. Solutions in

DMSO may be stored at -20°C for up to 3 months.

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