

YW3-56 (hydrochloride)

08/19

ALTERNATE NAMES: N-[(1S)-4-[(2-chloro-1-iminoethyl)amino]-1-[[(phenylmethyl)amino]carbonyl]butyl]-6-(dimethylamino)-2-

naphthalenecarboxamide, monohydrochloride

CATALOG #: B2858-500 500 μg B2858-1000 1000 μg

STRUCTURE:

MOLECULAR FORMULA: C₂₇H₃₂CIN₅O₂.HCl

MOLECULAR WEIGHT: 530.49

FORMULATION: A solution in methanol

PURITY: ≥80%

DESCRIPTION: YW3-56 is an inhibitor of protein arginine deiminases PAD2 and PAD4 which convert protein arginine

residues to citrulline. The IC $_{50}$ for inhibition of PAD4 and PAD2 is about 1–2 μ M and 0.5–1 μ M respectively. YW3-56 inhibits the growth of osteosarcoma U2OS cells with an IC $_{50}$ of 2.5 μ M. YW3-56 induces p53 target genes SESN2 and DDIT4 which repress mTORC1 kinase activity. It perturbs autophagy and inhibits the growth of triple-negative breast cancer xenograft tumors in mice.

STORAGE TEMPERATURE: -20°C

HANDLING: Do not take internally. Wear gloves and mask when handling the product! Avoid contact by all modes of

exposure.

REFERENCE: 1. Wang, Y., Li, P., Wang, S., et al. Anticancer peptidylarginine deiminase (PAD) inhibitors regulate the

autophagy flux and the mammalian target of rapamycin complex 1 activity. The Journal of Biological

Chemisty 287(31), 25941-25952 (2012).

2. Wang, S., Chen, X.A., Hu, J., et al. ATF4 gene network mediates cellular response to the anticancer PAD

inhibitor YW3-56 in triple-negative breast cancer cells. Mol. Cancer Ther. 14(4), 877-888 (2015).

RELATED PRODUCTS:

F-Amidine (trifluoroacetate salt) (Cat. No. B2803) GSK-199 hydrochloride (Cat. No. B1037) BB-Cl-Amidine (Cat. No. B2847)

CI-Amidine (hydrochloride) (Cat. No. B2802) GSK-121 trifluoroacetate (Cat. No. B1034)

DISCLAIMER: FOR RESEARCH USE ONLY! Not to be used on humans.