

Product Data Sheet

Product Name: ML161
Cat. No.: GC13004

Chemical Properties

Cas. No. 423735-93-7

Chemical Name 2-bromo-N-[3-(butanoylamino)phenyl]benzamide

SMILES CCCC(=O)NC1=CC=CC(=C1)NC(=O)C2=CC=CC=C2Br

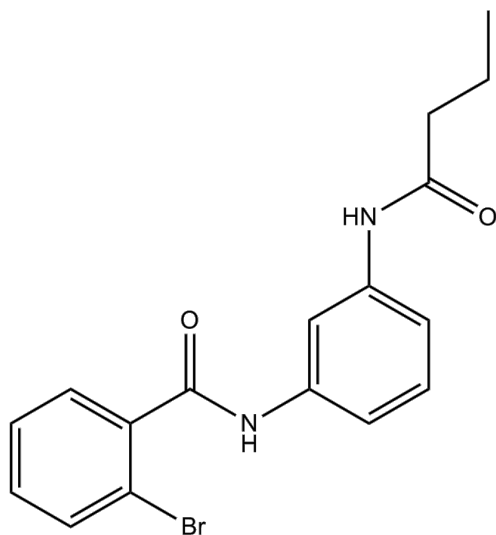
Formula $C_{17}H_{17}BrN_2O_2$ M.Wt 361.23

Solubility $\geq 16.4\text{mg/mL}$ in DMSO, $\geq 46.9\text{mg/mL}$ in EtOH with ultrasonic 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

ML161 is a selective inhibitor of PAR1 with IC_{50} value of $0.26\ \mu\text{M}$ [1].

Protease-activated receptor-1 (PAR-1) is a unique G-protein-coupled receptor belonging to the

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protease-activated receptor family and its activation leads to downstream signaling events that launch a variety of cellular responses related to tumor progression [1].

ML161 is a potent PAR1 inhibitor and has a different selectivity with the reported ALK inhibitor crizotinib. When tested with human platelets, ML161 treatment inhibited the activation of thrombin-induced platelet in a dose-dependent manner by detecting P-selectin expression [1]. When tested with granule secretion, ML161 exhibited a potent inhibition on P-selectin expression in a dose-dependent manner with EC50 value of 0.3 μ M and also inhibited SFLLRN-induced thrombus formation [2].

References:

- [1]. Dockendorff, C., et al., Discovery of 1,3-Diaminobenzenes as Selective Inhibitors of Platelet Activation at the PAR1 Receptor. ACS Med Chem Lett, 2012. 3(3): p. 232-237.
- [2]. VerPlank, L., et al., Chemical Genetic Analysis of Platelet Granule Secretion-Probe 3, in Probe Reports from the NIH Molecular Libraries Program. 2010, National Center for Biotechnology Information (US): Bethesda (MD).

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