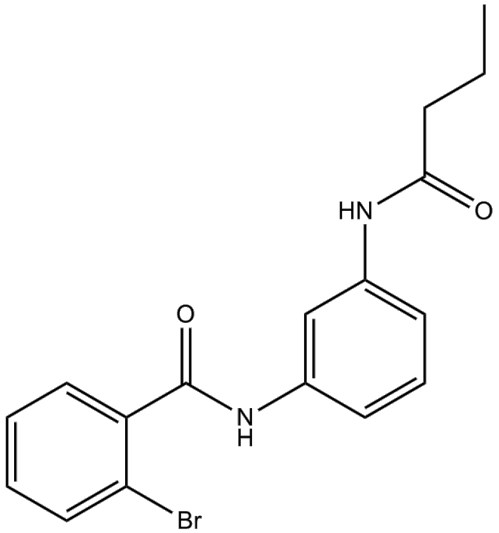
Product Data Sheet

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	≥ 16.4mg/mL in DMSO, ≥ 46.9 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 IC50 value of 0.26 μM [1].

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

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 0.3μM 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).