Certificate of Analysis

Product Name: **BPTU** **Catalog No.: 6078** **Batch No.: 1**

CAS Number: 870544-59-5

IUPAC Name: *N*-[2-[2-(1,1-Dimethylethyl)phenoxy]-3-pyridinyl]-*N*'-[4-(trifluoromethoxy)phenyl]urea

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{22}F_3N_3O_3$

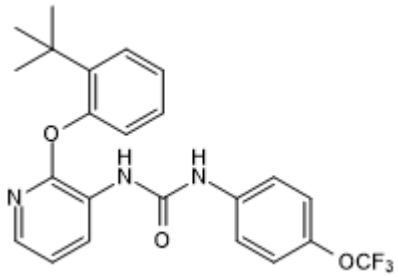
Batch Molecular Weight: 445.43

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.71 (50% Ethyl acetate:Petroleum ether)

HPLC: Shows >99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.02	4.98	9.43
Found	62.23	4.91	9.43

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Product Information

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Description:

Allosteric antagonist of $P2Y_1$ (EC_{50} = 0.06-0.3 μM). Non-nucleotide ligand. Binds receptor outside of the helical bundle. Blocks inhibition of spontaneous contraction of rat and mouse colon induced by electrical field stimulation, nicotine and P2Y agonists. Antithrombotic; reduces platelet aggregation.

Physical and Chemical Properties:

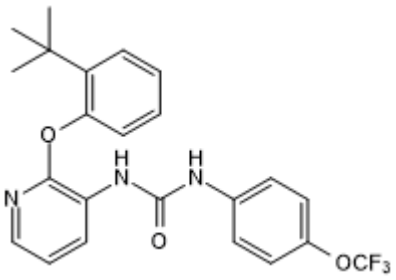
Batch Molecular Formula: $C_{23}H_{22}F_3N_3O_3$

Batch Molecular Weight: 445.43

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at RT

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Mañé *et al* (2016) BPTU, an allosteric antagonist of P2Y1 receptor, blocks nerve mediated inhibitory neuromuscular responses in the gastrointestinal tract of rodents. Neuropharmacology. ***2016*** 376. PMID: 27496690.

Zhang *et al* (2015) Two disparate ligand-binding sites in the human P2Y1 receptor. Nature. ***2015*** 317. PMID: 25822790.

Chao *et al* (2013) Discovery of 2-(phenoxypyridine)-3-phenylureas as small molecule P2Y1 antagonists. J.Med.Chem. ***2013*** 1704. PMID: 23368907.

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