Product Data Sheet

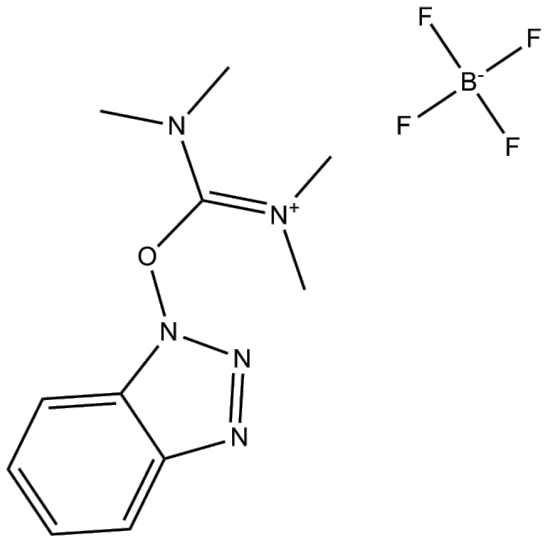
Product Name: TBTU

Cat. No.: GA10095

Chemical Properties

Cas No.	125700-67-6		
化学名	[benzotriazol-1-yloxy(dimethylamino)methylidene]-dimethylazanium;tetrafluoroborate		
Canonical SMILES	[B-](F)(F)(F)F.CN(C)C(=[N+](C)C)ON1C2=CC=CC=C2N=N1		
分子式	$C_{11}H_{16}BF_4N_5O$	分子量	321.1
溶解度	≥ 106mg/mL in DMSO, ≥ 50.2mg/mL in Water, <5.11mg/mL in EtOH	储存条件	Desiccate at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ 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

IC50: Not available.

The utilization of new peptide coupling reagents in organic synthesis has greatly flourished the development of peptide synthesis. TBTU, 2-(1H-Benzotriazol-1-yl)-1,1,3,3-tetramethyluronoium hexafluorphosphate, serves as a typical peptide coupling reagent which has a relatively lower racemization. In normal condition, coupling reactions mediated by TETU take only six minutes to complete when HOBt is added. Moreover, racemization in this reaction could be reduced to insignificant levels. Due to these features, TBTU is regarded as one of the key reagents of choice

Tel: (626) 353-8530 Fax: (626) 353-8530 E-mail: tech@glpbio.com
Address: 10292 Central Ave. #205, Montclair, CA, USA

in both manufactory and lab. [1]

In vitro: It was reported that during synthesis of the macrocyclic peptide cyclotheonamide B, TBTU played an important role in coupling steps. Studies showed that TBTU had been successfully used in several coupling reactions, for instance, this reagent was suitable for couplings involving proline nitrogen, and therefore served as a crucial reagent for the macrolactamization. Although TBTU normally proceeded with little racemization, to suppress the racemization completely, HOBt was also required. Thus, in a typical reaction system, TBTU was added into 0.5 mM solution of CH_2Cl_2, followed by addition of HOBt and pyridine. Finally, cyclopentapeptide was obtained with a yield of 61%. [1]

In vivo: So far, no in vivo data has been reported.

Clinical trial: So far, no clinical trial has been conducted.

Reference:
[1]Bastiaans HM, van der Baan JL and Ottenheijm HC. Flexible and convergent total synthesis of cyclotheonamide B. J. Org. Chem. 1997; 62: 3880-9.