Product Data Sheet

Product Name: TBTU
Cat. No.: GA10095

Chemical Properties

Cas. No.	125700-67-6		
Chemical Name	[benzotriazol-1-yloxy(dimethylamino)methylidene]-dimethylazanium;tetrafluoroborate		
SMILES	[B-](F)(F)(F)F.CN(C)C(=[N+](C)C)ON1C2=CC=CC=C2N=N1		
Formula	$C_{11}H_{16}BF_4N_5O$	M.Wt	321.1
Solubility	≥ 106mg/mL in DMSO, ≥ 50.2mg/mL in Water, <5.11mg/mL in EtOH	Storage	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	TBTU		

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 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

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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.