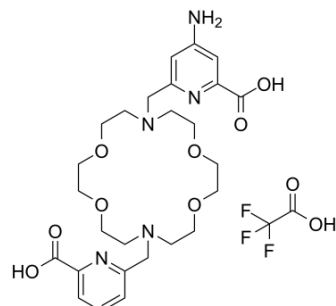


## Macropa-NH2 TFA

Cat. No.:	HY-111895B
Molecular Formula:	C <sub>28</sub> H <sub>38</sub> F <sub>3</sub> N <sub>5</sub> O <sub>10</sub>
Molecular Weight:	661.62
Target:	Others
Pathway:	Others
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



### SOLVENT & SOLUBILITY

In Vitro	DMSO : 200 mg/mL (302.29 mM; Need ultrasonic)				
		Solvent Concentration	Mass		
	Preparing Stock Solutions		1 mg	5 mg	10 mg
		1 mM	1.5114 mL	7.5572 mL	15.1144 mL
5 mM		0.3023 mL	1.5114 mL	3.0229 mL	
	10 mM	0.1511 mL	0.7557 mL	1.5114 mL	
Please refer to the solubility information to select the appropriate solvent.					
In Vivo	1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 5 mg/mL (7.56 mM); Clear solution  2. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 5 mg/mL (7.56 mM); Clear solution				

### BIOLOGICAL ACTIVITY

Description	Macropa-NH2 TFA is the precursor of Macropa-NCS. Macropa-NCS is conjugated to trastuzumab as well as to the prostate-specific membrane antigen-targeting compound RPS-070 and is a promising therapeutic radionuclide applied in the treatment of soft-tissue metastases <sup>[1]</sup> .
In Vitro	A white suspension of 11•4TFA (0.1598 g, 0.16 mmol) and Na <sub>2</sub> CO <sub>3</sub> (0.2540 g, 2.4 mmol) was heated at reflux in acetone (10 mL) for 30 min before the slow addition of CSCI <sub>2</sub> (305 μL of CSCI <sub>2</sub> , 85%, Acros Organics). The resulting orange suspension was heated at reflux for 3 h and then concentrated at 30 °C under reduced pressure to a pale-orange solid. The solid was dissolved portionwise in 10% ACN/H <sub>2</sub> O containing 0.2% TFA (8 mL total), filtered, and immediately purified by preparative HPLC using Method C. Pure fractions were combined, concentrated at RT under reduced pressure to remove the organic solvent, and then lyophilized. Fractions that were not able to be concentrated immediately were frozen at -80 °C. Isothiocyanate 12 was obtained as a mixture of white and pale-yellow solid (0.0547 g) and was stored at -80 °C in a jar of

Drierite. A stock solution containing 4.4 mg/mL of macropa-NCS was prepared in 0.1 M pH 9.1 NaHCO<sub>3</sub> buffer containing 0.154 M NaCl and was stored at -80 °C. To a portion of Tmab in saline (74 µL) were added macropa-NCS (52 µL) and NaHCO<sub>3</sub> buffer (266 µL), so that the final concentrations of Tmab and macropa-NCS were 5.1 mg/mL and 0.59 mg/mL, respectively. Macropa-NCS was estimated to be in 16-fold molar excess to Tmab based on a molecular weight of 1045.76 g/mol for macropa-NCS (tetra-TFA salt)<sup>[1]</sup>.

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

## REFERENCES

[1]. Thiele NA, et al. An Eighteen-Membered Macrocyclic Ligand for Actinium-225 Targeted Alpha Therapy. *Angew Chem Int Ed Engl.* 2017;56(46):14712-14717.

**Caution: Product has not been fully validated for medical applications. For research use only.**

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