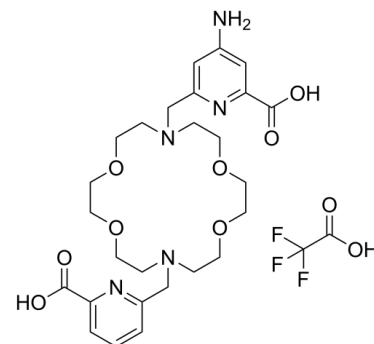


## Data Sheet

<b>Product Name:</b>	Macropa-NH2 (TFA)
<b>Cat. No.:</b>	CS-0136667
<b>CAS No.:</b>	2705054-08-4
<b>Molecular Formula:</b>	C <sub>28</sub> H <sub>38</sub> F <sub>3</sub> N <sub>5</sub> O <sub>10</sub>
<b>Molecular Weight:</b>	661.62
<b>Target:</b>	Others
<b>Pathway:</b>	Others
<b>Solubility:</b>	H <sub>2</sub> O : 100 mg/mL (ultrasonic); DMSO : ≥ 130 mg/mL



### BIOLOGICAL ACTIVITY:

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>.

### 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.

### CAIndexNames:

2,2,2-Trifluoroacetic acid compound with 4-amino-6-((16-((6-carboxypyridin-2-yl)methyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecan-7-yl)methyl)picolinic acid (1:1)

### SMILES:

O=C(O)C1=NC(CN2CCOCCOCCN(CC3=NC(C(O)=O)=CC=C3)CCOCCOCC2)=CC(N)=C1.O=C(O)C(F)(F)F

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

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