Macropa-NH2 hydrochloride

Cat. No.: HY-111895A

CAS No.: 2443966-86-5

Molecular Formula: $C_{26}H_{38}ClN_5O_8$

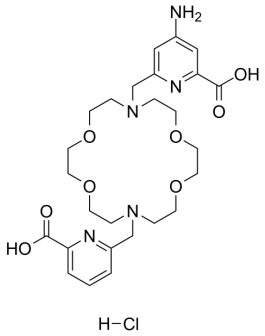
Molecular Weight: 584.06

Target: Others

Pathway: Others

Storage: 4°C, sealed storage, away from moisture

* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

H_2O : ≥ 100 mg/mL (171.22 mM)

DMSO : 83.33 mg/mL (142.67 mM; Need ultrasonic)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Concentration \ Solvent \ Mass	1 mg	5 mg	10 mg
1 mM	1.7122 mL	8.5608 mL	17.1215 mL
5 mM	0.3424 mL	1.7122 mL	3.4243 mL
10 mM	0.1712 mL	0.8561 mL	1.7122 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (3.56 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (3.56 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (3.56 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Macropa-NH2 hydrochloride is the precursor of Macropa-NCS. Macropa-NCS is conjugated to Anti-Human HER2 (HY-P9907) 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[1].

In Vitro

A white suspension of 11•4TFA (0.1598 g, 0.16 mmol) and Na2CO3 (0.2540 g, 2.4 mmol) was heated at reflux in acetone (10 mL) for 30 min before the slow addition of CSCl2 (305 µL of CSCl2, 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/H2O 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 NaHCO3 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 NaHCO3 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)[1].

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

CUSTOMER VALIDATION

- J Nucl Med. 2021 Aug 12;jnumed.121.262459.
- Sci Rep. 2020 Dec 17;10(1):22203.
- Patent. US20210236667A1.

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REFERENCES

[1]. Thiele NA, et al. An Eighteen-Membered Macrocyclic Ligand for Actinium-225 Targeted Alpha Therapy. Angew Chem Int Ed Engl. 2017 Nov 13;56(46):14712-14717.

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