

Product Name: VUF 11222

Catalog No.: 5668

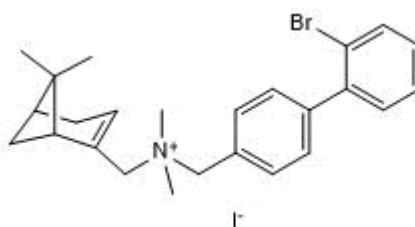
Batch No.: 1

CAS Number: 1414376-84-3

IUPAC Name: 2'-Bromo-*N*-[[[(1*R*,5*S*)-6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl]methyl]-*N,N*-dimethyl-[1,1'-biphenyl]-4-methanaminium iodide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₅ H ₃₁ BrIN
Batch Molecular Weight:	552.33
Physical Appearance:	Pale yellow solid
Solubility:	DMSO to 100 mM ethanol to 10 mM with gentle warming
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

TLC:	R _f = 0.04 (Ethyl acetate:Petroleum ether [3:17])
HPLC:	Shows 98.4% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	54.36	5.66	2.54
Found	54.5	5.71	2.65

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

High affinity non-peptide CXCR3 agonist ($pK_i = 7.2$).

Physical and Chemical Properties:

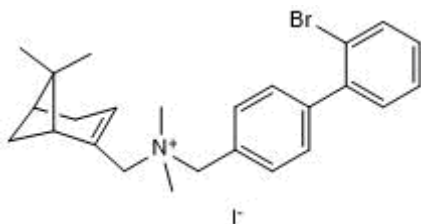
Batch Molecular Formula: $C_{25}H_{31}BrIN$

Batch Molecular Weight: 552.33

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 mM with gentle warming

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Wijtmans et al (2012) Chemical subtleties in small-molecule modulation of peptide receptor function: the case of CXCR3 biaryl-type ligands. *J.Med.Chem.* **55** 10572. PMID: 23150943.

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