Print Date: Dec 16th 2016

Certificate of Analysis

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Product Name: **ML 154** **Catalog No.: 5161** **Batch No.: 1**

CAS Number: 1345964-89-7

IUPAC Name: 3-(Diphenylphosphinothioyl)-2-methyl-1-[(2*E*)-3-phenyl-2-propen-1-yl]imidazo[1,2-*a*]pyridinium bromide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{29}H_{26}N_2PS.Br$

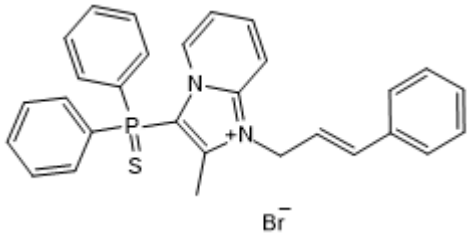
Batch Molecular Weight: 545.47

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.45 (Dichloromethane:Methanol [9:1])

HPLC: Shows 99.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.85	4.8	5.14
Found	63.91	4.73	5.12

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Product Information

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CAS Number: 1345964-89-7

IUPAC Name: 3-(Diphenylphosphinothioyl)-2-methyl-1-[(2*E*)-3-phenyl-2-propen-1-yl]imidazo[1,2-*a*]pyridinium bromide

Description:

Potent neuropeptide S receptor (NPSR) antagonist (pA_2 = 9.98). Inhibits neuropeptide S-induced ERK phosphorylation over cAMP responses and calcium responses (IC_{50} values are 9.3, 22.1 and 36.5 nM, respectively). Appears to modulate addictive behavior in vivo. Displays no activity against vasopressin V_{1B} receptors. Brain penetrant.

Physical and Chemical Properties:

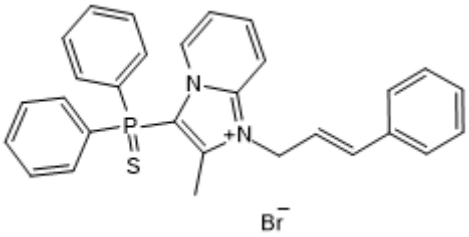
Batch Molecular Formula: $C_{29}H_{26}N_2PS.Br$

Batch Molecular Weight: 545.47

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 50 mM

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:

Patnaik *et al* (2013) Structure-activity relationship of imidazopyridinium analogues as antagonists of neuropeptide s receptor. J Med Chem. ***56*** 9045. PMID: 24171469.

Thorsell *et al* (2013) A novel brain penetrant NPS receptor antagonist, NCGC00185684, blocks alcohol-induced ERK-phosphorylation in the central amygdala and decreases operant alcohol self-administration in rats. J.Neurosci. ***33*** 10132. PMID: 23761908.

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