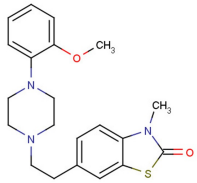
Data Sheet (Cat.No.T10168)

TargetMol
A DRUG SCREENING EXPERT

5-HT1A modulator 1

Chemical Properties



CAS No.:	142477-34-7
Formula:	C21H25N3O2S
Molecular Weight:	383.51
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	5-HT1A modulator 1 displays very high affinities for the 5HT1A, adrenergic α1, and dopamine D2 receptor (IC50s: 2 nM, 10 nM and 40 nM).
Targets(IC_{50})	sPLA2: 2 nM 5-HT1B Receptor: 300 nM 5-HT2A Receptor: 500 nM 5-HT2C Receptor: 4000 nM α1 receptor: 10 nM D2 receptor: 40 nM
In vivo	5-HT1A modulator 1 (Compound 24) shows clear antagonist action at 5HT2A receptor subtype in mice. The antagonism is nearly complete at the dose of 1 mg/kg i.p for 5-HT1A modulator 1 (94% of antagonism). 5-HT1A modulator 1 completely blocks the stereotypies and the climbing at the dose of 1 mg/kg i.p (100% of antagonism). 5-HT1A modulator 1 is also tested in rats, using the same paradigm. After oral administration, 5-HT1A modulator 1 significantly reduces the hyperactivity by 50% at the doses of 2 and 4 mg/kg p.o, respectively 63% and 58% of antagonism for 5-HT1A modulator 1; the antagonism is complete (103% and 108%) at the respective doses of 8 and 16 mg/kg p.o for 5-HT1A modulator 1.
Kinase Assay	Binding is determined using membranes prepared from the bovine hippocampus. The receptor is labeled with 0.5 nM [3H]-8-hydroxydipropylaminotetralin (8-OH-DPAT) by incubation at 25°C for 30 min with 11 concentrations of the test compounds (1-10^5 nM). Nonspecific binding is determined using 10 μM buspirone. Competition experiments are analyzed using the iterative nonlinear least-squares curve-fitting program Inplot 4, GraphPad; IC50 values are calculated using the Cheng-Prusoff equation.

Solubility Information

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.607 mL	13.037 mL	26.075 mL
5 mM	0.521 mL	2.607 mL	5.215 mL
10 mM	0.261 mL	1.304 mL	2.607 mL
50 mM	0.052 mL	0.261 mL	0.521 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Taverne T, et al. Novel benzothiazolin-2-one and benzoxazin-3-one arylpiperazine derivatives with mixed 5HT1A/D2 affinity as potential atypical antipsychotics. J Med Chem. 1998 Jun 4;41(12):2010-8.

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