

Product Data Sheet

Product Name: ML314
Cat. No.: GC18216

Chemical Properties

Cas. No. 1448895-09-7

Chemical Name 2-cyclopropyl-6,7-dimethoxy-4-[4-(2-methoxyphenyl)-1-piperazinyl]-quinazoline

SMILES COC1=C(OC)C=C(C(N2CCN(C3=CC=CC=C3OC)CC2)=NC(C4CC4)=N5)C5=C1

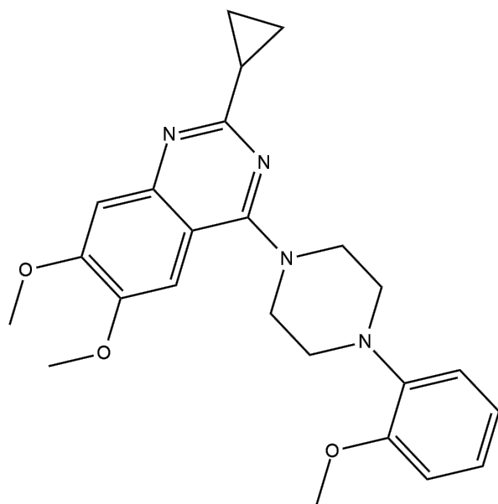
Formula $C_{24}H_{28}N_4O_3$ M.Wt 420.5

Solubility DMSO: >100mM Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Background

ML314 is a potent molecule agonist of NTR1 ($EC_{50} = 1.9 \mu M$); showed good selectivity against NTR2 and GPR35, but did not stimulate Ca^{2+} mobilization. IC_{50} value: $1.9 \mu M$ (EC_{50}) [1] Target: NTR1 agonist. Medicinal chemistry optimization of MLS-0233108 led to ML314, the most potent molecule in this second series that exhibited full agonist behavior (100 %) on NTR1 ($EC_{50} = 1.9 \mu M$).

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

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com

Address: 10292 Central Ave. #205, Montclair, CA, USA

Product Data Sheet

ML314 showed good selectivity against NTR2 and GPR35, but did not stimulate Ca²⁺ mobilization. ML314 is potentially a biased agonist operating via the β -arrestin pathway rather than the traditional Gq coupled pathway. Signaling mediated by β -arrestin has distinct biochemical and functional consequences that may lead to physiological advantages as described below. This probe report describes the discovery and properties of ML301 and summarizes the HTS and follow-up campaign, which identified ML314.

References:

[1]. Hershberger P, et al. Small Molecule Agonists for the Neurotensin 1 Receptor (NTR1 Agonists). Probe Reports from the NIH Molecular Libraries Program

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

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com

Address: 10292 Central Ave. #205, Montclair, CA, USA