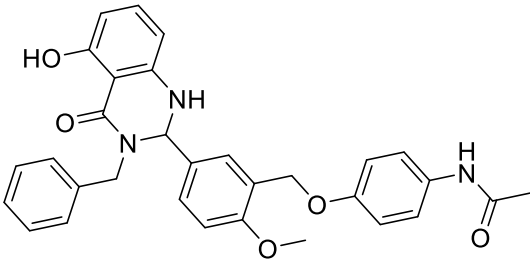


Product data sheet



MedKoo Cat#: 555782 Name: ML109 CAS#: 1186649-91-1 Chemical Formula: C ₃₁ H ₂₉ N ₃ O ₅ Exact Mass: 523.2107 Molecular Weight: 523.59		
Product supplied as:	Powder	
Purity (by HPLC):	≥ 98%	
Shipping conditions	Ambient temperature	
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years. In solvent: -80°C 3 months; -20°C 2 weeks.	

1. Product description:

ML-109, also known as CID-25246343, is a potent and full thyroid stimulating hormone receptor (TSHR) agonist. ML109 (CID-25246343) is the first selective and orally available small-molecule TSHR agonist, and the probe will be a useful pharmacological tool to study TSHR biology in thyroidal and extrathyroidal tissues.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under “QC And Documents” section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	83.0	158.5

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.91 mL	9.55 mL	19.10 mL
5 mM	0.38 mL	1.91 mL	3.82 mL
10 mM	0.19 mL	0.95 mL	1.91 mL
50 mM	0.04 mL	0.19 mL	0.38 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of “Calculator”

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Titus S, Huang W, Marugan J, Southall N, Inglese J, Austin C, Zheng W, Englund E, Neumann S, Gershengorn M. Identification of Potent and Selective Thyroid Stimulating Hormone Receptor Agonists. 2009 Sep 1 [updated 2011 Mar 25]. In: Probe Reports from the NIH Molecular Libraries Program [Internet]. Bethesda (MD): National Center for Biotechnology Information (US); 2010-. PMID: 21735603.

In vivo study

1. Titus S, Huang W, Marugan J, Southall N, Inglese J, Austin C, Zheng W, Englund E, Neumann S, Gershengorn M. Identification of Potent and Selective Thyroid Stimulating Hormone Receptor Agonists. 2009 Sep 1 [updated 2011 Mar 25]. In: Probe Reports from the NIH Molecular Libraries Program [Internet]. Bethesda (MD): National Center for Biotechnology Information (US); 2010-. PMID: 21735603.

7. Bioactivity

Biological target:

ML-109 is a potent and full thyroid stimulating hormone receptor (TSHR) agonist with an EC₅₀ of 40 nM.

Product data sheet



In vitro activity

The effects of CID-25246343/ML109 or TSH on cAMP accumulation in cells expressing TSHR, TSHR-KFLR in which the large amino-terminal ectodomain to which TSH binds, is deleted, or N5.47A in which Asn at position-5.47 was mutated to Ala. Docking of CID-25246343/ML109 into the homology model of TSHR predicts CID-25246343/ML109 binds within the transmembrane helical bundle (left panel). Enlargement of the boxed region in the left panel (right panel) shows an interaction of CID-25246343/ML109 with an Asn in TMH5 (N5.47). CID-25246343/ML109 activates TSHR by binding to the transmembrane helical bundle.

Reference: National Center for Biotechnology Information (US); 2010. <https://pubmed.ncbi.nlm.nih.gov/21735603/>

In vivo activity

Vehicle (PEG 300, control) or CID-25246343/ML109 (2.5 mg) was given by esophageal gavage and serum T4 was measured 2 hr later. Vehicle (control) or CID-25246343/ML109 (2.5 mg) was given by esophageal gavage on days 1 and 2. On the morning of the 3rd day, Na¹²⁵I (20 μ Ci) was administered by esophageal gavage and the mice were sacrificed 2 hr later. The thyroid glands and small pieces of liver were excised and counted for ¹²⁵I radioactivity. These in vivo studies (Figure 6) showed that CID-25246343/ML109 could increase secretion of T4 and thyroidal iodide uptake in mice after administration by esophageal gavage, suggesting CID-25246343/ML109 is an orally available small molecule that can stimulate thyroid gland function.

Reference: National Center for Biotechnology Information (US); 2010. <https://pubmed.ncbi.nlm.nih.gov/21735603/>

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.