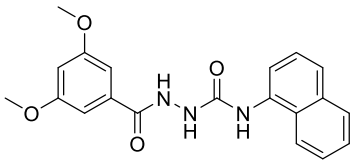
Product data sheet

MedKoo Cat#: 530602 Name: TC-O9311 CAS#: 444932-31-4 Chemical Formula: $C_{20}H_{19}N_3O_4$ Exact Mass: 365.1376 Molecular Weight: 365.39	
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:
TC-O9311 is a potent GPR139 agonist (EC50 = 39 nM in CHO-K1 cells expressing human GPR139).

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	14	38.32
DMF	11	30.10
Ethanol	14	38.32
PBS (pH 7.2)	5	13.68

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	2.74 mL	13.68 mL	27.37 mL
5 mM	0.55 mL	2.74 mL	5.47 mL
10 mM	0.27 mL	1.37 mL	2.74 mL
50 mM	0.05 mL	0.27 mL	0.55 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

TBD

In vivo study

Shi et al (2011) Discovery and SAR of a series of agonists at orphan G protein-coupled receptor 139. ACS Med.Chem.Lett. 2 303

7. Bioactivity
Biological target:

TC-O 9311 is a potent GPR139 agonist

In vitro activity

TBD

Product data sheet

In vivo activity

A screening campaign identified compound 1a as a high potency GPR139 agonist with an EC50 = 39 nM in a calcium mobilization assay in CHO-K1 cells stably expressing the GPR139 receptor. In the absence of a known endogenous ligand, the maximum effect was set as 100% for 1a. Screening against 90 diverse targets revealed no cross-reactivity issues. Assessment of the pharmacokinetic properties showed limited utility as in vivo tool compound in rat with a poor whole brain exposure of 61 ng/g and a brain/plasma (b/p) ratio of 0.03. Attempts to identify a more suitable analogue identified the des-nitrogen analogue 1s with a reduced polar surface area of 76.7 Å(2) and an improved b/p ratio of 2.8. The whole brain exposure remained low at 95 ng/g due to a low plasma exposure.

Reference: Shi et al (2011) Discovery and SAR of a series of agonists at orphan G protein-coupled receptor 139. ACS Med.Chem.Lett. 2 303