

Product Name: YIL 781 hydrochloride

Catalog No.: 3959

Batch No.: 3

CAS Number: 1640226-17-0

IUPAC Name: 6-(4-Fluorophenoxy)-2-methyl-3-[[[(3S)-1-(1-methylethyl)-3-piperidiny]methyl]-4(3H)-quinazolinone hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₈FN₃O₂.HCl.¾H₂O

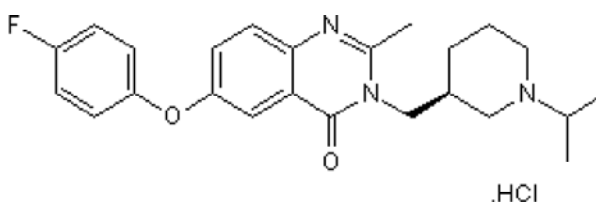
Batch Molecular Weight: 459.47

Physical Appearance: Tan solid

Solubility: DMSO to 100 mM
ethanol to 100 mM
water to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.26 (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.2% purity

Chiral HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	62.74	6.69	9.15	7.71
Found	62.71	6.67	8.94	8.01

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Ghrelin receptor antagonist (GHS-R1a) ($K_i = 17$ nM). Displays no significant affinity for the motilin receptor ($K_i = 6$ μ M). Blocks the effects of ghrelin on insulin secretion both in vivo and in vitro. Improves glucose homeostasis in vivo.

Physical and Chemical Properties:

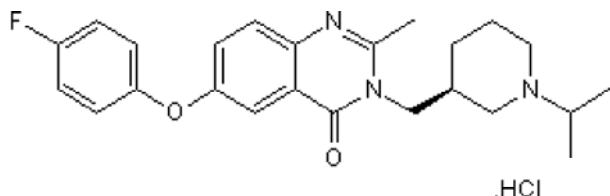
Batch Molecular Formula: $C_{24}H_{28}FN_3O_2 \cdot HCl \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 459.47

Physical Appearance: Tan solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 mM
water to 100 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:

Moran and Dailey (2009) Gut peptides: targets for antiobesity drug development? *Endocrinology* **150** 2526. PMID: 19372201.

Esler et al (2007) Small-molecule ghrelin receptor antagonists improve glucose tolerance, suppress appetite, and promote weight loss. *Endocrinology* **148** 5175. PMID: 17656463.

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