

Product Name: AR-C 141990 hydrochloride

Catalog No.: 5658

Batch No.: 1

IUPAC Name: 5-[[[(3*R*)-3-Hydroxy-1-pyrrolidinyl]carbonyl]-3-methyl-1-(2-methylpropyl)-6-(4-quinolinylmethyl)thieno[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₂₈N₄O₄S.HCl.H₂O

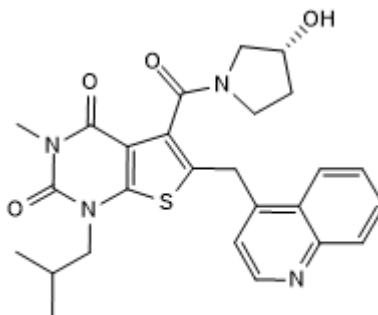
Batch Molecular Weight: 547.07

Physical Appearance: Pale yellow solid

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

Storage: Store at -20°C

Batch Molecular Structure:



HCl

2. ANALYTICAL DATA

TLC: R_f = 0.26 (Ethyl acetate:Methanol [92:8])

HPLC: Shows >99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.08	5.71	10.24
Found	57.02	5.59	10.21

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Description:

Monocarboxylate transporter (MCT1) inhibitor ($pK_i = 7.6$). Exhibits approximately 10-fold selectivity for MCT1 over MCT2 and no significant activity against MCT3 or 4. Inhibits graft versus host response and prolongs cardiac graft survival in a rat model. Immunosuppressant. Also inhibits brain penetration of GHB analog HOCPA.

Physical and Chemical Properties:

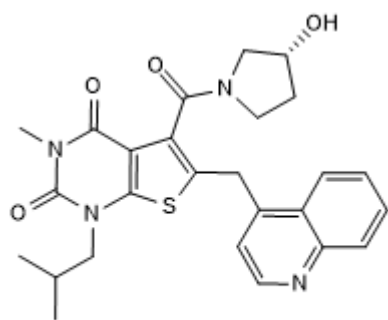
Batch Molecular Formula: $C_{26}H_{28}N_4O_4S.HCl.H_2O$

Batch Molecular Weight: 547.07

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



HCl

Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM

DMSO to 100 mM

ethanol 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:

Thiesen et al (2015) *In vitro* and *in vivo* evidence for active brain uptake of the GHB analog HOCPA by the monocarboxylate transporter subtype 1. *J.Pharmacol.Exp.Ther.* **354** 166. PMID: 25986445.

Pählman et al (2012) Immunosuppressive properties of a series of novel inhibitors of the monocarboxylate transporter MCT-1. *Transpl.Int.* **26** 22. PMID: 23137339.

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956