

Product Name: Chroman 1

Catalog No.: 7163

Batch No.: 1

IUPAC Name: (3*S*)-*N*-[2-[2-(Dimethylamino)ethoxy]-4-(1*H*-pyrazol-4-yl)phenyl]-3,4-dihydro-6-methoxy-2*H*-1-benzopyran-3-carboxamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₈N₄O₄·2HCl·1¼H₂O

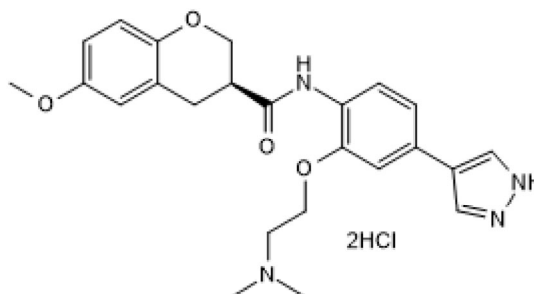
Batch Molecular Weight: 531.95

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
water to 5 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

Chiral HPLC: Shows 98.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	54.19	6.16	10.53	13.33
Found	54.81	6.44	10.61	11.8

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

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Description:

Chroman 1 is a highly potent and selective ROCK2 (Rho-kinase) inhibitor (IC₅₀ values are 1 and 52 pM at ROCK2 and ROCK1, respectively). Chroman 1 exhibits >2000-fold selectivity for ROCK2 over a range of related kinases including MRCK, PKA, and AKT1 (IC₅₀ values are 150, >20000, and >20000 nM, respectively). Chroman 1 promotes survival of pluripotent stem cells (PSCs) in culture when used in combination with Emricasan (Cat. No. 7310), Polyamine Supplement x1000 (lyophilized) (Cat. No. 7739), and Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

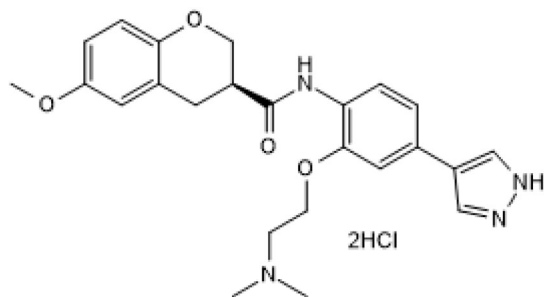
Batch Molecular Formula: C₂₄H₂₈N₄O₄·2HCl·1¼H₂O

Batch Molecular Weight: 531.95

Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Chen et al (2021) A versatile polypharmacology platform promotes cytoprotection and viability of human pluripotent and differentiated cells. *Nat.Methods* **18** 528. PMID: 33941937.

Chen et al (2011) Asymmetric synthesis of potent chroman-based Rho kinase (ROCK-II) inhibitors. *Med.Chem.Commun.* **2** 73.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

water to 5 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

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