Certificate of Analysis

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: $C_{24}H_{28}N_4O_4.2HCl.1¼H_2O$

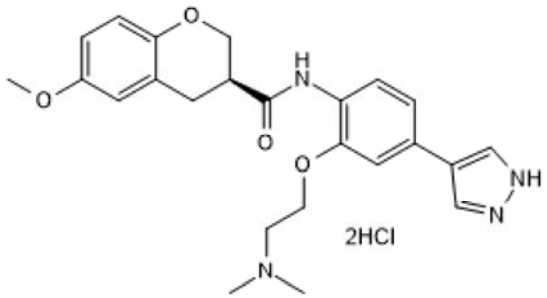
Batch Molecular Weight: 531.95

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

^{1}H 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

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Product Information

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Description:

Chroman 1 is a highly potent and selective ROCK2 (Rho-kinase) inhibitor (IC_{50} 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 (IC_{50} 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), Polyamines, and

Physical and Chemical Properties:

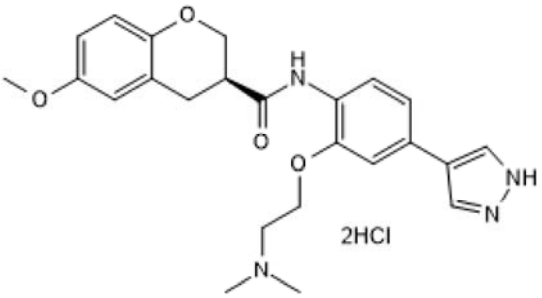
Batch Molecular Formula: $C_{24}H_{28}N_4O_4.2HCl.1¼H_2O$

Batch Molecular Weight: 531.95

Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:



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. 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:

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.