Certificate of Analysis

Product Name: **Ro 31-8220 mesylate** **Catalog No.: 2002** **Batch No.: 2**

CAS Number: 138489-18-6

IUPAC Name: 3-[3-[2,5-Dihydro-4-(1-methyl-1*H*-indol-3-yl)-2,5-dioxo-1*H*-pyrrol-3-yl]-1*H*-indol-1-yl]propyl carbamimidothioic acid ester mesylate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{23}N_5O_2S.CH_3SO_3H$

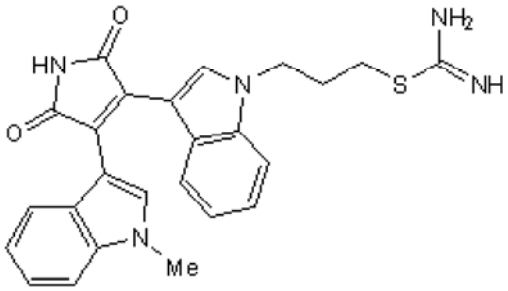
Batch Molecular Weight: 553.65

Physical Appearance: Orange solid

Solubility: DMSO to 100 mM
ethanol to 5 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

Melting Point: Between 244 - 248°C(dec)

HPLC: Shows 97.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.4	4.92	12.64
Found	56.25	4.97	12.44

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Description:

Protein kinase C inhibitor, with activity at other protein kinases (IC_{50} values are 33, 3, 8, 15 and 38 nM for PKCα, MAPKAP-K1b, MSK1, GSK3β and S6K1 respectively). Activates JNK and glycogen synthase, and inhibits MAPK and ERK2, in rat adipocytes and L6 myotubes. Also inhibits voltage-dependent Na^+ channels in the micromolar range. Induces protein-protein interaction between mutant $SMAD4^{R361H}$ and SMAD3, leading to reactivation of dormant $SMAD4^{R361H}$-mediated transcriptional activity and restoration of TGF-β-induced tumor suppression activity in SMAD4 mutant cancer cells.

Physical and Chemical Properties:

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Minimum Purity: ≥97%

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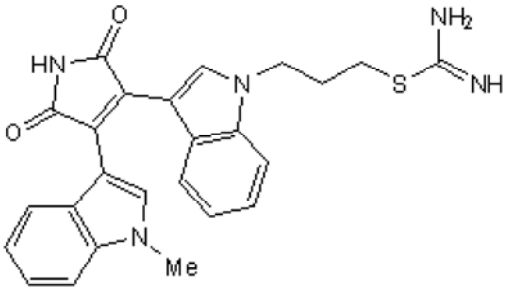

Storage: Desiccate at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Davies *et al* (2000) Specificity and mechanism of action of some commonly used protein kinase inhibitors. Biochem.J. ***351*** 95. PMID: 10998351.

Lingameneni *et al* (2000) Inhibition of voltage-dependent sodium channels by Ro 31-8220, a 'specific' protein kinase C inhibitor. FEBS Lett. ***473*** 265. PMID: 10812087.

Standaert *et al* (1999) RO 31-8220 activates c-Jun N-terminal kinase and glycogen synthase in rat adipocytes and L6 myotubes. Comparison to actions of Ins. Endocrinology ***150*** 2145.