Certificate of Analysis

Product Name: **PQ 69** **Catalog No.: 5351** **Batch No.: 1**

CAS Number: 910045-32-8

IUPAC Name: 4-(Butylamino)-2-(3-fluorophenyl)-1,2-dihydro-3*H*-pyrazolo[4,3-*c*]quinolin-3-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{19}FN_4O$

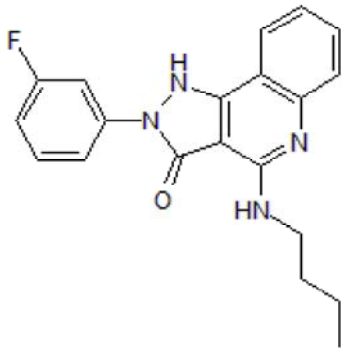
Batch Molecular Weight: 350.39

Physical Appearance: Orange solid

Solubility: DMSO to 100 mM
ethanol to 10 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.32 (Dichloromethane:Methanol [97:3])

HPLC: Shows 98.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.56	5.47	15.99
Found	68.64	5.34	15.93

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Description:

Potent and selective A_1 receptor inverse agonist. Exhibits high binding affinity at A_1 receptor (K_i values are 0.07 and 0.96 nM for rat and human receptors respectively). Reduces basal [^{35}S] -GTPγS binding 44.6% (IC_{50} = 0.19 nM). Antagonizes the effects of A_1 agonist R-PIA (IC_{50} = 18.3 nM) and exhibits competitive antagonism on CCPA-induced tracheal contractions ex vivo. Displays 217- fold selectively over hA_{2A} receptor and >1000-fold selectivity over hA_3 receptor.

Physical and Chemical Properties:

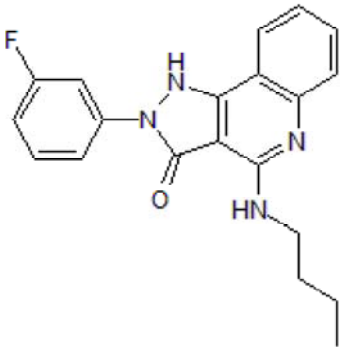
Batch Molecular Formula: $C_{20}H_{19}FN_4O$

Batch Molecular Weight: 350.39

Physical Appearance: Orange solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 10 mM with gentle warming

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:

Lu *et al* (2014) PQ-69, a novel and selective adenosine A_1 receptor antagonist with inverse agonist activity. Purinergic Signal. ***10*** 619. PMID: 25248972.