1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** $C_{20}H_{28}N_{6}O_{3} \cdot \frac{1}{4}H_{2}O$
- **Batch Molecular Weight:** 404.97
- **Physical Appearance:** White solid
- **Solubility:** DMSO to 100 mM, ethanol to 100 mM
- **Storage:** Store at -20°C

2. ANALYTICAL DATA

- **HPLC:** Shows 98.3% purity
- **$^1$H NMR:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Microanalysis:**
  - Theoretical: Carbon 59.32, Hydrogen 7.09, Nitrogen 20.75
  - Found: Carbon 59.23, Hydrogen 7.15, Nitrogen 20.94
Description:
cdk2 inhibitor (IC_{50} = 0.5 \, \mu M). Exhibits >8-fold selectivity for CDK2 over CDK1 and CDK4 (IC_{50} values are 4.2 and 215 \, \mu M, respectively). Inhibits proliferation rat neonatal aortic smooth muscle cells and a range of tumor cells lines in vitro. Inhibits restenosis in a rat carotid artery injury model.

Physical and Chemical Properties:
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Batch Molecular Weight: 404.97
Physical Appearance: White solid
Minimum Purity: >98%

References:

Storage: Store at -20°C
Solubility & Usage Info:
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.