1. PHYSICAL AND CHEMICAL PROPERTIES

- Batch Molecular Formula: $\text{C}_{13}\text{H}_{10}\text{ClN}_{3}\text{O}$
- Batch Molecular Weight: 259.69
- Physical Appearance: Off White solid
- Solubility: DMSO to 100 mM
- Storage: Store at +4°C

2. ANALYTICAL DATA

- TLC: $R_f = 0.67$ (Ethyl acetate:Petroleum ether [1:2])
- HPLC: Shows 98.7% purity
- $^1\text{H NMR}$: Consistent with structure
- Mass Spectrum: Consistent with structure
- Microanalysis:
  - Carbon: Theoretical 60.13, Found 60.11
  - Hydrogen: Theoretical 3.88, Found 3.86
  - Nitrogen: Theoretical 16.17, Found 16.03
Product Name: Ro 5-3335
CAS Number: 30195-30-3
IUPAC Name: 7-Chloro-1,3-dihydro-5-(1H-pyrrol-2-yl)-2H-1,4-benzodiazepin-2-one

Description:
Core binding factor (CBF) inhibitor; preferentially kills human leukemia cell lines with CBF fusion proteins (IC_{50} = 1.1 μM). Represses RUNX1/CBFβ-dependent transactivation in reporter assays and inhibits transcriptional regulation by RUNX1 and CBFβ. Reduces leukemia burden in a mouse model. Attenuates RUNX1-dependent hematopoiesis in zebrafish embryos. Also a Tat antagonist; inhibits HIV-1 replication in vitro.

Physical and Chemical Properties:
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Minimum Purity: >98%

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Solubility & Usage Info:
DMSO 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.

References: