

Certificate of Analysis

Print Date: Jul 19th 2019

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Product Name: KS 176 Catalog No.: 4169 Batch No.: 1

CAS Number: 1253452-78-6

IUPAC Name: N-[4-(2-Hydroxyethyl)phenyl]-2-[(4-nitrobenzoyl)amino]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

 $C_{22}H_{19}N_3O_5$ **Batch Molecular Formula:**

Batch Molecular Weight: 405.4

Off-white solid **Physical Appearance:**

DMSO to 100 mM Solubility: Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.6$ (Ethyl acetate) **HPLC**: Shows 98.7% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 65.18 4.72 10.37 Found 65 4.69 10.51



Product Information

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IUPAC Name: N-[4-(2-Hydroxyethyl)phenyl]-2-[(4-nitrobenzoyl)amino]benzamide

Description:

Selective inhibitor of the breast cancer resistance protein (BCRP) multidrug transporter (IC $_{50}$ values are 0.59 and 1.39 μ M in Pheo A and Hoechst 33342 assays respectively). Displays no inhibitory activity against P-gp or MRP1.

Physical and Chemical Properties:

 $\begin{array}{l} \text{Batch Molecular Formula: } C_{22}H_{19}N_3O_5 \\ \text{Batch Molecular Weight: 405.4} \end{array}$

Physical Appearance: Off-white solid

Batch Molecular Structure:

Minimum Purity: >98%

Storage: Store at +4°C

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:

Pick et al (2010) Specific inhibitors of the breast cancer resistance protein (BCRP). ChemMedChem 5 1498. PMID: 20632361.

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