



# **Certificate of Analysis**

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Product Name: CC 0651 Catalog No.: 4503 Batch No.: 1

CAS Number: 1319207-44-7

IUPAC Name: (2R,3S,4S)-5-[4-(3,5-Dichlorophenyl)phenyl]-2,3-dihydroxy-4-(2-methoxyacetamido)pentanoic acid

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{20}H_{21}CI_2NO_6$ 

Batch Molecular Weight: 442.29

Physical Appearance: Off White solid

Solubility: 1eq. NaOH to 100 mM

DMSO to 100 mM ethanol to 50 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.3$  (Dichloromethane:Methanol [4:1])

HPLC: Shows 98.8% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 54.31 4.79 3.17 Found 54.7 4.75 3.16



## **Product Information**

Print Date: May 27<sup>th</sup> 2016

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#### **Description:**

Allosteric inhibitor of human Cdc34. Inhibits hCdc34-mediated ubiquitination of p27<sup>Kip1</sup> (IC $_{50}$  = 1.72  $\mu$ M). Exhibits selectivity for hCdc34 over Uba1, Ube2G1, UbcH7, UbcH5, Ube2N (Ubc13), Ube2R2, SMURF2, SspH1 and Rnf168.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>20</sub>H<sub>21</sub>Cl<sub>2</sub>NO<sub>6</sub> Batch Molecular Weight: 442.29 Physical Appearance: Off White solid

Minimum Purity: >98%

#### **Batch Molecular Structure:**

Storage: Store at -20°C

#### Solubility & Usage Info:

1eq. NaOH to 100 mM DMSO to 100 mM ethanol to 50 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:

**Huang** et al (2014) E2 enzyme inhibition by stabilization of a low-affinity interface with ubiquitin. Nat.Chem.Biol. **10** 156. PMID: 24316736.

Ceccarelli et al (2011) An allosteric inhibitor of the human Cdc34 ubiquitin-conjugating enzyme. Cell 145 1075. PMID: 21683433.