Print Date: Aug 22nd 2018

Certificate of Analysis

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Product Name: **(R)-CE3F4** **Catalog No.: 5969** **Batch No.: 1**

CAS Number: 1593478-56-8

IUPAC Name: (2*R*)-5,7-Dibromo-6-fluoro-3,4-dihydro-2-methyl-1(2*H*)-quinolinecarboxaldehyde

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{11}H_{10}Br_2FNO$

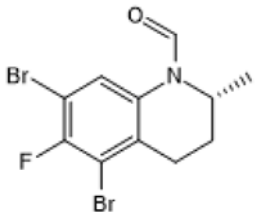
Batch Molecular Weight: 351.01

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.33 (20% EtOAc/petrol)

HPLC: Shows 99.7% purity

Chiral HPLC: Shows >99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -14.3 (Concentration = 1, Solvent = Chloroform)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	37.64	2.87	3.99
Found	37.76	2.81	3.9

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Description:

Epac inhibitor (IC_{50} values are 4.2 and 44 µM for Epac1 and Epac2(B), respectively). Blocks activation of Epac by cAMP. This is the R-enantiomer of CE3F4 (Cat.No.4793).

Physical and Chemical Properties:

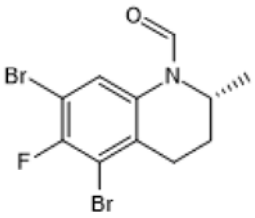
Batch Molecular Formula: $C_{11}H_{10}Br_2FNO$

Batch Molecular Weight: 351.01

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

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.

Licensing Information:

Sold for research use only under license from Inserm, Université Toulouse III - Paul Sabatier, Université Paris-Sud and Université d'Orléans.

References:

Boulton *et al* (2018) Mechanism of selective enzyme inhibition through uncompetitive regulation of an allosteric agonist. J.Am.Chem.Soc. ***140*** 9624. PMID: 30016089.

Courilleau *et al* (2013) The (*R*)-enantiomer of CE3F4 is a preferential inhibitor of human exchange protein directly activated by cyclic AMP isoform 1 (Epac1). Biochem.Biophys.Res.Commun. ***440*** 443. PMID: 24099776.

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