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Certificate of Analysis

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Product Name: ZE 132

Catalog No.: 7533 Batch No.: 1

CAS Number: 2566710-63-0

IUPAC Name:

2-[[[5-Chloro-2-[(5-cyano-3-pyridinyl)methoxy]-4-[[3-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-methylphenyl]methoxy] phenyl]methyl][3-(dimethylamino)propyl]amino]ethanesulfonic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage:

Batch Molecular Structure:

 $C_{37}H_{41}CIN_4O_7S.2^{1/2}H_2O$ 766.31 White solid DMSO to 100 mM Store at -20°C



2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: Microanalysis: Shows 98.2% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 57.99 6.05 7.31 Found 57.82 5.67 7.26

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

IUPAC Name:

ZE 132 binds to programmed cell death-ligand 1 (PD-L1) with high affinity (K_D = 19.36 nM); it potently and selectively inhibits the interaction between programmed cell death-1 (PD-1) and PD-L1 (IC_{50} = 23.49 nM). ZE 132 promotes CD8⁺ T cell activation and improves the in vitro cytotoxic killing activity of T-cells. ZE 132 treatment can increase Cxcl9 mRNA expression and lower Tgfb1 mRNA expression in CT26 mouse colorectal cancer model. ZE 132 shows antitumor effects, inhibiting growth of CT26 tumors in mice by 64%.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{37}H_{41}CIN_4O_7S.2^{1/2}H_2O$ Batch Molecular Weight: 766.31 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Liu *et al* (2021) Discovery of a novel, potent and selective small-molecule inhibitor of PD-1/PD-L1 interaction with robust *in vivo* anti-tumour efficacy. Br.J.Pharmacol. **178** 2651. PMID: 33768523.

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Storage: Store at -20°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 $45-60^{\circ}C$ 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.