

Certificate of Analysis

Print Date: Aug 16th 2022

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Product Name: STING agonist C53 Catalog No.: 7741 Batch No.: 1

CAS Number: 2259624-71-8

IUPAC Name: 1-[(2-Chloro-6-fluorophenyl)methyl]-2,3-dihydro-3,3-dimethyl-2-oxo-*N*-[(2,4,6-trifluorophenyl)methyl]-1*H*-indole-6-

carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{19}CIF_4N_2O_2$

Batch Molecular Weight: 490.88 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 61.17 3.9 5.71 Found 61.09 3.88 5.63



Product Information

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Description:

STING agonist C53 is an activator of human STING (EC $_{50}$ = 185 nM). It promotes the oligomerization and activation of human STING through a mechanism orthogonal to that of cGAMP. STING agonist C53 increases activity of STING variants in HEK293T cells (107%, 92% and 92% reporter activity against H232, R232 and HAQ, respectively). It induces phosphorylation of STING variants in human tumor cell lines and PBMCs. STING agonist C53 is active at human but not mouse STING. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₅H₁₉CIF₄N₂O₂

Batch Molecular Weight: 490.88 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

F N CI N

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°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:

Lu et al (2022) Activation of STING by targeting a pocket in the transmembrane domain. Nature 604 557. PMID: 35388221.

Pryde et al (2021) The discovery of potent small molecule activators of human STING. Eur.J.Med.Chem. 209 112869. PMID: 33038794.