

Certificate of Analysis

Print Date: Apr 6th 2023

www.tocris.com

Product Name: MD13 Catalog No.: 7503 Batch No.: 1

CAS Number: 2758431-97-7

IUPAC Name: 8-((2-(2,6-Dioxopiperidin-3-yl)-1,3-dioxoisoindolin-4-yl)amino)-N-(4-(7-hydroxy-2-oxo-2H-benzo[e][1,3]oxazin-3(4H)-

yl)phenyl)octanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₅H₃₅N₅O₈.H₂O

Batch Molecular Weight: 671.71

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 62.58 5.55 10.43 Found 62.52 5.49 10.32



Product Information

Print Date: Apr 6th 2023

www.tocris.com

Product Name: MD13 Catalog No.: 7503 1

CAS Number: 2758431-97-7

IUPAC Name: 8-((2-(2,6-Dioxopiperidin-3-yl)-1,3-dioxoisoindolin-4-yl)amino)-N-(4-(7-hydroxy-2-oxo-2H-benzo[e][1,3]oxazin-3(4H)-

yl)phenyl)octanamide

Description:

MD13 is a potent MIF (macrophage migration inhibitory factor) Degrader (PROTAC®) (DC₅₀ < 100 nM; D_{max} = 92% after 6 h). MD13 comprises the cereblon ligand Pomalidomide (Cat. No. 6302) joined by a linker to a MIF inhibitor. MD13 reduces MIF levels, arrests cells at the G_2/M phase and inhibits proliferation of A549 lung carcinoma cells. Growth of A549 cell 3D spheroids is also inhibited by MD 13. Negative control MD15 (Cat.No. 7504) also available. PROTAC® is a registered trademark of Arvinas Operations, Inc., and is used under license. Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

Batch Molecular Formula: C₃₅H₃₅N₅O₈.H₂O

Batch Molecular Weight: 671.71 Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:

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.

Licensing Information:

Sold with kind permission of Professor Dekker.

References:

Xiao et al (2021) Proteolysis targeting chimera (PROTAC) for macrophage migration inhibitory factor (MIF) has anti-proliferative activity in lung cancer cells. Angew.Chem.Int.Ed.Engl. 60 17514. PMID: 34018657.

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