bio-techne
TOCRIS

Print Date: Apr 6th 2023

Certificate of Analysis

www.tocris.com

Product Name: **MS 39** **Catalog No.: 7397** **Batch No.: 1**

CAS Number: 2675490-92-1

IUPAC Name: (2*S*,4*R*)-1-((*S*)-2-(11-(4-(3-((4-((3-Chloro-4-fluorophenyl)amino)-7-methoxyquinazolin-6-yl)oxy)propyl)piperazin-1-yl)-11-oxoundecanamido)-3,3-dimethylbutanoyl)-4-hydroxy-*N*-(4-(4-methylthiazol-5-yl)benzyl)pyrrolidine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{55}H_{71}ClFN_9O_7S.½H_2O$

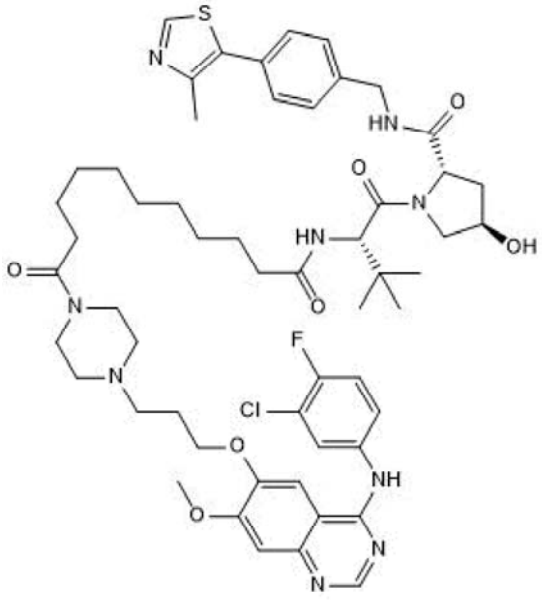
Batch Molecular Weight: 1065.75

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.99	6.81	11.83
Found	61.59	6.87	11.85

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Description:

MS 39 is a potent, high affinity and selective Degrader (PROTAC®) of mutant epidermal growth factor receptor (EGFR), comprising gefitinib (Iressa, Cat. No. 3000) conjugated via a linker to a VHL ligand. MS 39 potently induces degradation of mutant EGFR (DC_{50} values are 5 nM and 3.3 nM in HCC827 (exon 19 del) and H3255 (L858R mutation) lung cancer cell lines, respectively), but exhibits no significant effect in cell lines bearing wild-type EGFR at concentrations up to 10 µM. MS 39 inhibits proliferation of H3255 lung cancer cells in vitro, and is bioavailable in mice following ip administration. PROTAC® is a registered trade... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

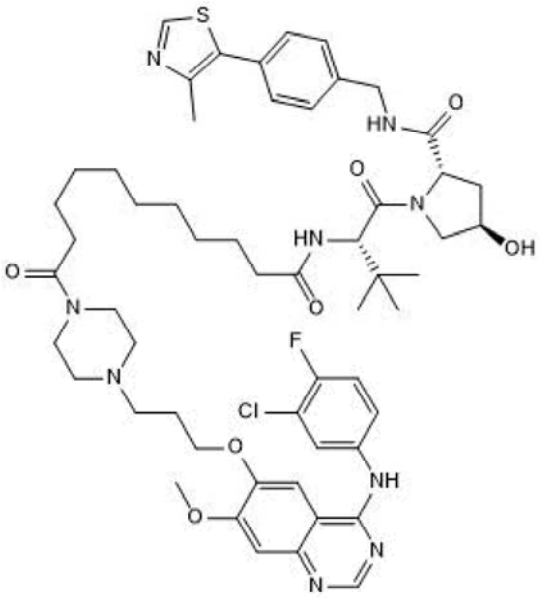
Batch Molecular Formula: $C_{55}H_{71}ClFN_9O_7S.½H_2O$

Batch Molecular Weight: 1065.75

Physical Appearance: White 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 under license from Icahn School of Medicine at Mount Sinai.

References:

Cheng *et al* (2020) Discovery of potent and selective epidermal growth factor receptor (EGFR) bifunctional small-molecule degraders. J.Med.Chem. ***63*** 1216. PMID: 31895569.