

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: C₅₅H₇₁ClFN₉O₇S.½H₂O

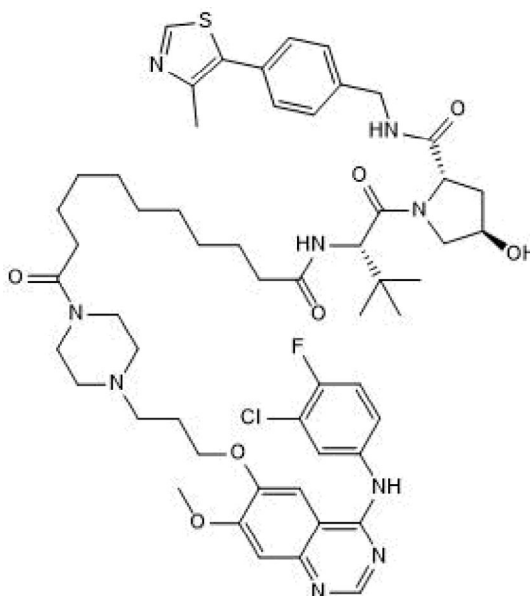
Batch Molecular Weight: 1065.75

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

¹H 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

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

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Description:

MS 39 is a potent, high affinity and selective Degradator (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 (DC₅₀ 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. EGFR antibody validated for Simple W... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

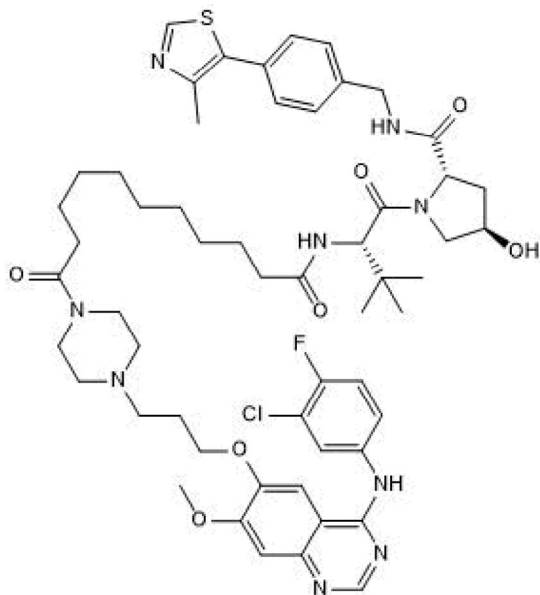
Batch Molecular Formula: C₅₅H₇₁ClFN₉O₇S.½H₂O

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel:+1 612 379 2956