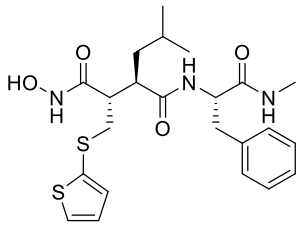
Product data sheet

MedKoo Cat#: 200442 Name: Batimastat CAS#: 130370-60-4 (free base) Chemical Formula: $C_{23}H_{31}N_3O_4S_2$ Exact Mass: 477.1756 Molecular Weight: 477.64	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
Batimastat (also known as BB-94) is a synthetic matrix metalloproteinase inhibitor that has shown antineoplastic and antiangiogenic activity in various tumor models. Matrix metalloproteinases (MMPs) are thought to play a significant role in tumor invasion and metastasis as well as angiogenesis. Batimastat, also known as BB-94, acts as an inhibitor of metalloproteinase activity by binding the zinc ion in the active site of MMPs.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	20.0	41.87
DMF	20.0	41.87

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.09 mL	10.47 mL	20.94 mL
5 mM	0.42 mL	2.09 mL	4.19 mL
10 mM	0.21 mL	1.05 mL	2.09 mL
50 mM	0.04 mL	0.21 mL	0.42 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Kirkegaard T, Yde CW, Kveiborg M, Lykkesfeldt AE. The broad-spectrum metalloproteinase inhibitor BB-94 inhibits growth, HER3 and Erk activation in fulvestrant-resistant breast cancer cell lines. Int J Oncol. 2014 Jul;45(1):393-400. doi: 10.3892/ijo.2014.2434. Epub 2014 May 9. PMID: 24819550.

In vivo study

1. Wu Z, Mulatibieke T, Niu M, Li B, Dai J, Ye X, He Y, Chen C, Wen L, Hu G. Inhibition of Matrix Metalloproteinase with BB-94 Protects against Caerulein-Induced Pancreatitis via Modulating Neutrophil and Macrophage Activation. Gastroenterol Res Pract. 2020 Apr 28;2020:8903610. doi: 10.1155/2020/8903610. PMID: 32411205; PMCID: PMC7204304.
2. Wang B, Liu D, Liu G, Zhang X, Wang Q, Zheng J, Zhou Y, He Q, Zhang L. Protective effects of batimastat against hemorrhagic injuries in delayed jellyfish envenomation syndrome models. Toxicon. 2015 Dec 15;108:232-9. doi: 10.1016/j.toxicon.2015.10.022. Epub 2015 Nov 4. PMID: 26546696.

7. Bioactivity
Biological target:

Product data sheet

Batimastat is a broad spectrum MMP inhibitor with IC50 of 3, 4, 4, 6, and 20 nM for MMP-1, MMP-2, MMP-9, MMP-7 and MMP-3, respectively.

In vitro activity

To further investigate the importance of HER receptors and HER ligand shedding for cell growth and signaling in the resistant cell lines, 164^R-7 was treated for five days with gefitinib (preferentially targeting EGFR), CI-1033 (pan-HER inhibitor), or the metalloproteinase inhibitors TAPI-2, BB-94 or GM6001 (Fig. 4A). Compared to growth of the untreated control, 1 μM gefitinib or 0.5 μM CI-1033 significantly inhibited growth of 164^R-7 by 30 and 80%, respectively. Moreover, the broad-spectrum metalloproteinase inhibitor BB-94 significantly inhibited resistant growth by 70%, whereas the more selective metalloproteinase inhibitors TAPI-2 and GM6001 had no inhibitory effect on growth of 164^R-7 (Fig. 4A). When the five-day dose-response growth experiments with BB-94 were performed, increasing concentrations (0.01–10 μM) of BB-94 resulted in a dose-dependent growth inhibition up to 50% and 80% compared to the untreated control for 164^R-7 and 164^R-5, respectively, whereas growth of the parental MCF-7 cells in the presence of increasing concentrations of BB-94 was <20% inhibited compared to the untreated control (Fig. 4B). Thus, BB-94 preferentially inhibited growth of fulvestrant-resistant MCF-7 cell lines.

Reference: Int J Oncol. 2014 Jul;45(1):393-400. https://www.spandidos-publications.com/ijo/45/1/393

In vivo activity

Firstly, using SR-based X-ray microangiography, this study found that TE did induce significant microvasculature alterations in hepatic and renal small vessel branches, especially in distal vessels as usual, while BB-94 significantly improved TE-induced hepatic and renal microvasculature changes in DJES mouse model. Secondly, under SR-μCT, TE also caused incomplete hepatic and renal distal vessel branches, while BB-94 reduced TE-induced hepatic and renal microvasculature changes in DJES rat model. In addition, being consistent with imaging results, histopathological and TUNEL-like staining observations also clearly corroborated this hypothesis, as BB-94 was highly effective in neutralizing TE-induced extensive hemorrhage and necrosis in DJES rat model. Taken together with previous findings, present data suggested that TE contained some metalloproteinases, which disrupted the integrity of microvasculars, resulting in liver and kidney hemorrhagic injuries in DJES, while rapid administration of BB-94 was useful in preventing TE-induced microvasculature alterations and appeared to be a promising therapeutic alternative for the treatment of DJES.

Reference: Toxicon. 2015 Dec 15;108:232-9. https://pubmed.ncbi.nlm.nih.gov/26546696/