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## Product Data Sheet

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Product Name: Calpain Inhibitor XII

Cat. No.: GC12479

**Chemical Properties**

Cas. No. 181769-57-3

Chemical Name [3-methyl-1-[[[1-[oxo[(2-pyridinylmethyl)amino]acetyl]butyl]amino]carbonyl]butyl]-carbamic acid, phenylmethyl ester

SMILES O=C(NC(CC(C)C)C(NC(CCC)C(C(NCC1=NC=CC=C1)=O)=O)=O)OCC2=CC=CC=C2Formula  $C_{26}H_{34}N_4O_5$  M.Wt 482.6Solubility  $\leq 16\text{mg/ml}$  in ethanol;  $16\text{mg/ml}$  in DMSO;  $20\text{mg/ml}$  in dimethyl formamide Storage Store at  $-20^\circ\text{C}$ 

General tips For obtaining a higher solubility, please warm the tube at  $37^\circ\text{C}$  and shake it in the ultrasonic bath for a while. Stock solution can be stored below  $-20^\circ\text{C}$  for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available sizes: ship with RT, or blue ice upon request.

Structure **Background**Ki: 19 nM for  $\mu$ -calpain

Calpain Inhibitor XII is a reversible and selective inhibitor of calpain I.

Calpain is a protein belonging to the family of calcium-dependent, non-lysosomal cysteine proteases expressed ubiquitously in mammals and many other organisms. Calpain inhibitors have been used to study the role of calpains in diverse processes, including neutrophil chemotaxis, neuronal signaling, and cardiac response to injury.

In vitro: A series of new dipeptidyl alpha-keto amides of the general structure R1-L-Leu-D,L-AA-CONH-R2 including Calpain Inhibitor XII were synthesized and evaluated as inhibitors for the cysteine proteases calpain I, calpain II, and cathepsin B. Calpain II was more sensitive to these inhibitors Calpain Inhibitor XII than calpain I. Calpain I was also effectively inhibited by Calpain Inhibitor XII, but lower Ki values than with calpain II. Cathepsin B was weakly inhibited by Calpain Inhibitor XII. The best calpain I inhibitor in this study was Calpain

**Caution: Product has not been fully validated for medical applications. For research use only.**

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Inhibitor XII with Ki value of 19 nM [1].

In vivo: Up to now, there is no animal in vivo data reported.

Clinical trial: So far, no clinical study has been conducted.

Reference:

[1] Li, Z. ,Ortega-Vilain, A.C.,Patil, G.S., et al. Novel peptidyl  $\alpha$ -keto amide inhibitors of calpains and other cysteine proteases. Journal of Medicinal Chemistry 39(20), 4089-4098 (1996).

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