Specificities of Binding of Different Inhibitors of Cahepsins

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Thiol protease Cathepsins play a significant role in proteolysis especially in certain desease states in humans. Mode of inhibition by different protein inhibitors in not clear yet. Keeping this in mind modeling studies were initiated with previously known and reently identified inhibitors of stefin family with intact and truncated n-terminal inhibitor. We find that role of N- terminal wedge as well as the second hairpin loop is very important. Inhibition mechanism also differs for endo and exo peptidase.

Keywords: thiol protease, cathepsins, stefins