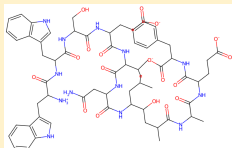
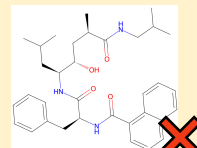
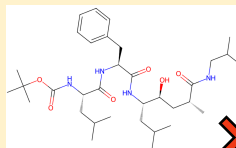
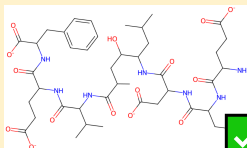


Question: Can this molecule bind to the BACE1 protein?



Input Molecule



Few-shot Example

<think>

Step 1: Molecular Structure Analysis

The target molecule is a complex **heptapeptide containing multiple tryptophan residues** (Cc1c2c([nH]c1)cccc2), **leucine/isoleucine branched side chains**, **glutamate carboxylates** ([O-]), and both N-terminal amino and C-terminal carboxyl functionalities. The peptide backbone provides extensive amide hydrogen bonding capability, while the aromatic indole rings offer π - π stacking interactions. The molecule adopts an extended conformation due to steric interactions between bulky side chains.

Step 2: Chemical Principle Application

BACE1 accommodates peptide substrates with specific P1-P4 binding subsites, particularly favoring hydrophobic residues at P1 and P3 positions for optimal cleavage. The **calculated molecular weight approximately 1200 Da exceeds typical small molecule inhibitors but matches endogenous peptide substrates**. The multiple tryptophan residues can form favorable π - π interactions with Phe108 and Tyr71 in the BACE1 active site, while the peptide backbone enables **key hydrogen bonds with catalytic Asp32 and Asp228 residues**. The extended structure spans the bilobal enzyme cleft effectively.

Step 3: Few-shot Comparative Analysis

The "True" example shares critical peptide characteristics: **multiple amide bonds, charged termini, and aromatic side chains distributed throughout the sequence**. Both "False" examples are shorter peptides with fewer aromatic residues and limited conformational flexibility for optimal active site engagement. Our target molecule exhibits **superior structural complexity with dual tryptophan residues providing enhanced binding interactions compared to the single phenylalanine in negative examples**. The extended peptide length matches the "True" example's capacity for multi-point enzyme contact.

Conclusion:

Optimal peptide length + favorable aromatic interactions + structural similarity to positive substrate + appropriate backbone flexibility for enzyme cleft binding indicates effective BACE1 recognition and binding.

<answer>True</answer>