

**DATASHEET**

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**HIV gag peptide (199-207)****Cat. No.:** RP20251**Size:** 1 mg**Description:**

Using a strain of *Listeria monocytogenes* that stably expresses and secretes HIV gag to deliver this Ag to the MHC class I pathway of Ag processing, we have identified the immunodominant CTL epitope to gag in the BALB/c mouse and shown that it is Kd restricted. The specific motif for the peptides that bind the MHC class I molecule H-2 Kd is believed to be a nonamer with residues tyrosine or phenylalanine in the second amino acid position and leucine or isoleucine in the carboxyl-terminal or ninth amino acid position as dominant anchoring positions. Surprisingly, the identified gag peptide, AMQMLKETI, does not contain an anchoring aromatic residue in position two although competition assays with other Kd-restricted epitopes indicated that it binds to Kd with comparable affinity. Using a theoretical molecular dynamics approach to probe the stability of peptide binding to MHC class I molecules, we show that the absence of an appropriate anchor residue at P2 in AMQMLKETI is compensated by favorable interactions of the glutamine at P3 with pocket D of Kd. These findings were verified experimentally, demonstrating the predictive power of this theoretical approach in analyzing MHC class I/peptide interactions. These studies also indicate that CTL epitope prediction that relies on dominant peptide motifs may not always identify the correct epitope.

**Sequence (one-letter code):**

AMQMLKETI

**Sequence (three-letter code):**

{Ala}{Met}{Gln}{Met}{Leu}{Lys}{Glu}{Thr}{Ile}

**Formula:** C<sub>45</sub>H<sub>81</sub>N<sub>11</sub>O<sub>14</sub>S<sub>2</sub>**Molecular Weight:** 1,064.33**Note:**

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