

研究论文

计算机辅助筛选酪氨酸激酶相关蛋白TRP-2 CTL模拟表位

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摘要 运用多项式方案、量化基序方案等经典的CTL表位筛选方案, 初步筛选了酪氨酸激酶相关蛋白TRP-2 CTL表位TRP-2_{180~188} (SVYDFVWL)的模拟表位, 以通过表位改造提高其与HLA-A2.1分子结合的能力, 从而提高其免疫原性. 根据打分结果, 合成了4个得分较高的九肽序列, 亲和力实验结果表明所筛选的4个序列较原序列均有较高的亲和力, 但对2位的单突变结果较1和2位双突变结果理想, 进一步运用分子模拟方法对4个序列与HLA-A2.1分子间的相互作用进行了分子模拟分析, 分子模拟结果较好地解释了上述实验现象, 从而为进一步的结构改造提供了理论依据. 本研究提供了一个合理高效的模拟表位筛选方法.

关键词 [酪氨酸激酶相关蛋白](#) [模拟表位](#) [分子模拟](#)

分类号

Computer Aided Screening of Tyrosinase Related Protein-2 (180~188) Mimotope

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Abstract To enhance HLA-A2.1 molecule affinity and immunogenicity of the tyrosinase related protein-2 (180~188) epitope, the classical epitope prediction methods including the polynomial method and the quantitative motif method were used to predict the modified epitope. Then four altered peptide ligands (APLs) with high score were synthesized, and their affinity with HLA-A2.1 molecule was assayed. The results show that the four APLs have high affinity, but the results of single mutant at P2 are better than those of double mutant at P1 and P2. So the molecular modeling was performed to study the interaction between the APLs and HLA-A2 molecule, and the results give a rational reason for the experimental results and provide the theoretical base for the further structure modification. This study provides a rational and high efficiency method to screen mimotope.

Key words [tyrosinase related protein-2](#) [mimotope](#) [molecular modeling](#)

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