**Novel anticancer peptide inhibits cancer progression by blocking Hsp90 factor: An *in­ Silico* study**

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**Introduction**: Anticancer peptides (ACPs) are small peptides, often derived from natural peptides. Various cationic peptides show extensive cytotoxicity against different cancer cells. Hsp90 is a chaperone, which plays a crucial role in development of a wide range of proteins. Blocking the function of Hsp90 causes degradation of the oncogenic proteins, leading to the control of the growth of cancer. Therefore, aim of the present study is design the anticancer peptide as possible peptide drug molecule for Hsp90 targeting through *in silico* analysis.

**Methods:** In this study, we have extracted 100 experimentally un-benchmark anticancer peptides from databases (<http://aps.unmc.edu/AP/>). Anticancer activity for each peptide estimated with iACP software and sequences with high anticancer activity was selected. Then, one sequence submits to AntiCP server for design of newly anticancer peptides. The 3D model of peptide was created with I-TASSER software. The Pdb structures of peptides were docked with the Hsp90α using Hex 6.1 and the peptide with the maximum binding energy value was identified.

**Results:** About 400 peptides with anticancer property, design in AntiCP server. Anticancer activity of new design peptides with higher score in AntiCP displayed 98-99.9% anticancer specificity. Result of this study showed that among the various screened peptides, KRGLAYKKKFQARGKKFAKKLAKKL identified as potential sequence for Hsp90α factor.

**Conclusion:** result in this study indicated that the probability of successful design of novel anticancer peptide. Therefore, our designed peptide can be used as potential anticancer drugs against cancer cells.

**Key words**: Anticancer peptides, Hsp90, in silico, cancer development