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Molecular Evaluation of RNase from *Aspergillus niger* and Phytol of *Nymphaea pubescens* as Cytoskeletol targeting elements in Cancer

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The aim of the present research was to study the anticancer effects of Aspergillus niger (A.niger) RNase and Phytol of *Nymphaea pubescens*. We found that RNase (A.niger RNase) and Phytol significantly and dose dependently inhibited invasiveness of breast cancer cell line MDA MB 231 by 55 % ($P<0.01$) at 1 μM concentration. At a concentration of 2 μM, the anti invasive effect of the enzyme increased to 90% ($P<0.002$). Keeping the aim to determine molecular level interactions (molecular simulations and protein docking) of human actin with A.niger RNase and Phytol of *Nymphaea pubescens*. We extended our work in-vitro to in-silico studies. To gain better relaxation and accurate arrangement of atoms, refinement was done on the human actin and A.niger RNase and Phytol of *Nymphaea pubescens* by energy minimization (EM) and molecular dynamics (MD) simulations using 43A2 force field of Gromacs96 implemented in the Gromacs 4.0.5 package, finally the interaction energies were calculated by protein-protein, protin-ligand docking using the HEX and autodock respectively. These in-vitro and in-silico structural studies prove the effective inhibition of actin activity by A.niger RNase Phytol of *Nymphaea pubescens* in neoplastic cells and thereby provide new insights for the development of novel anti cancer drugs.

Keywords: A. niger RNase, Phytol of *Nymphaea pubescens*, Anticancer therapeutics, cancer celllines, Gromacs 4.0.5, HEX server, Human actin, Protein docking

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