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Potential anticancer peptides design from the cysteine rich plant defensins: An *in silico* approach

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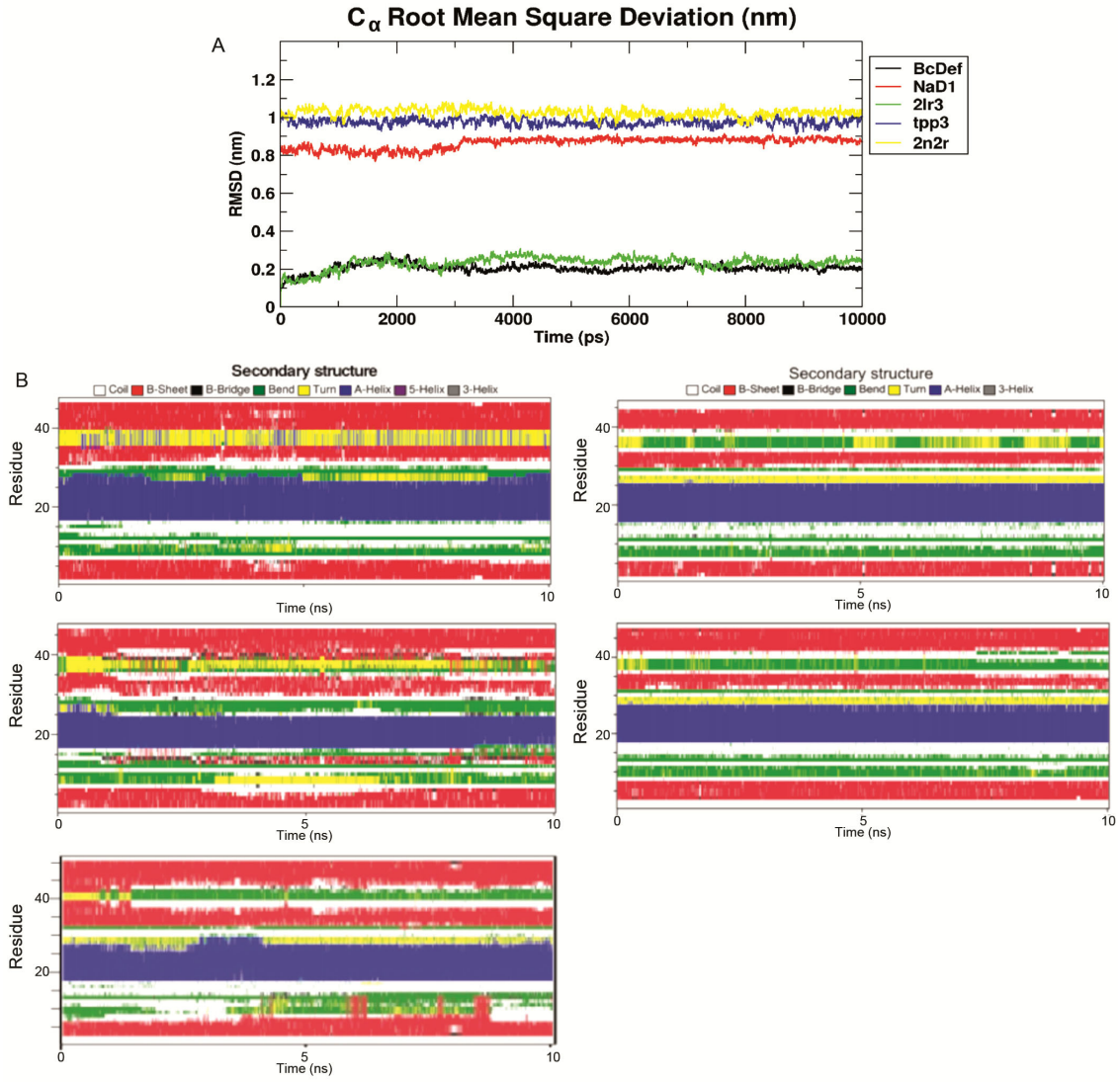
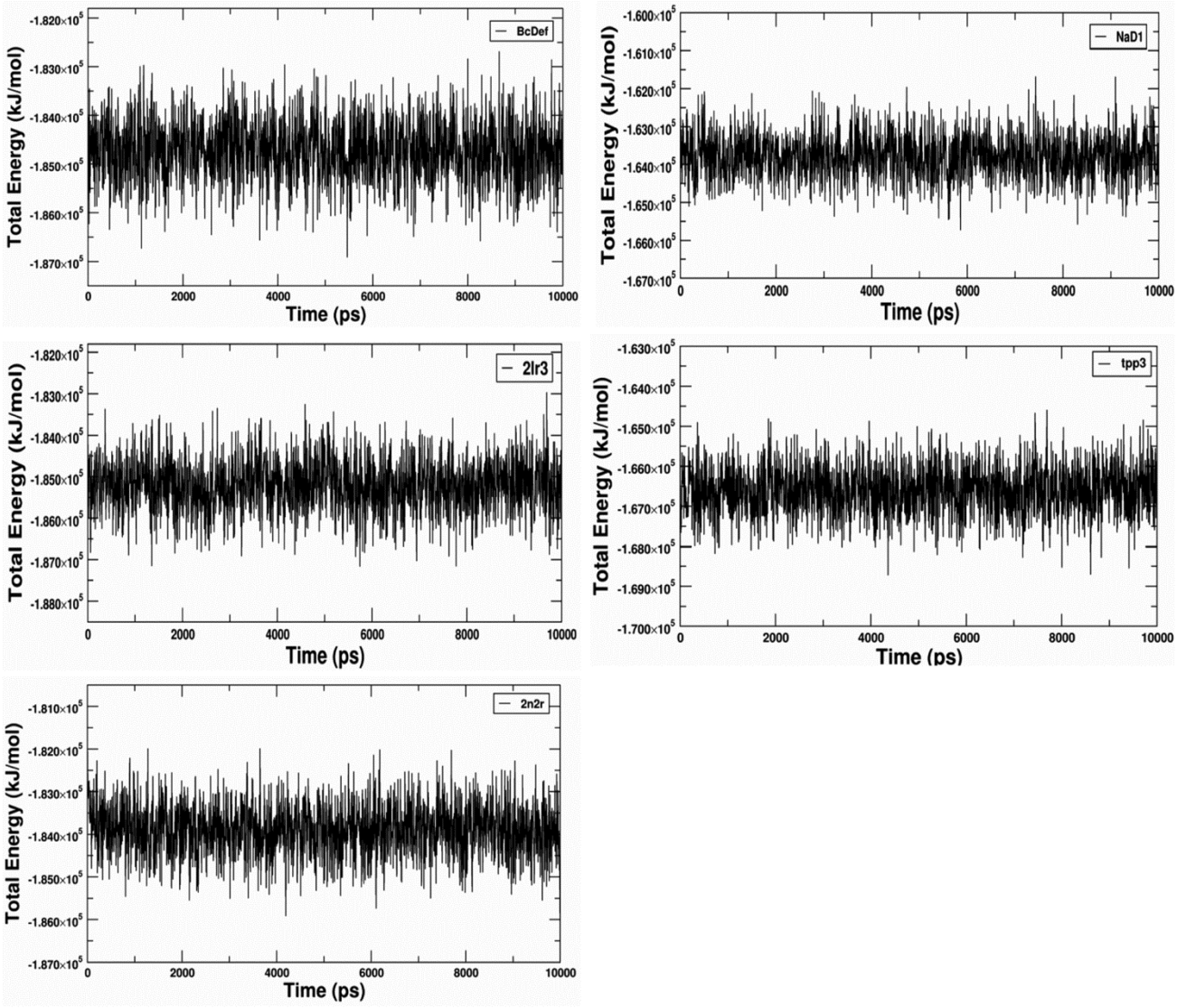
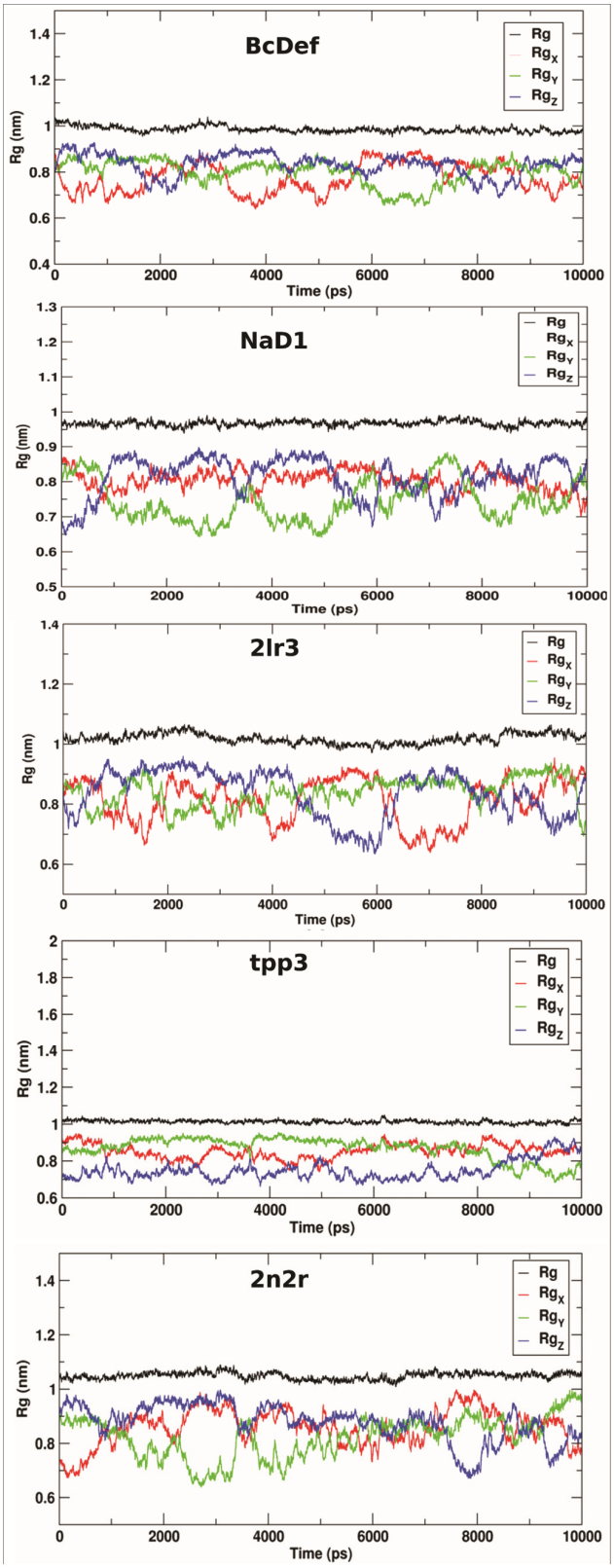
Supplementary Data



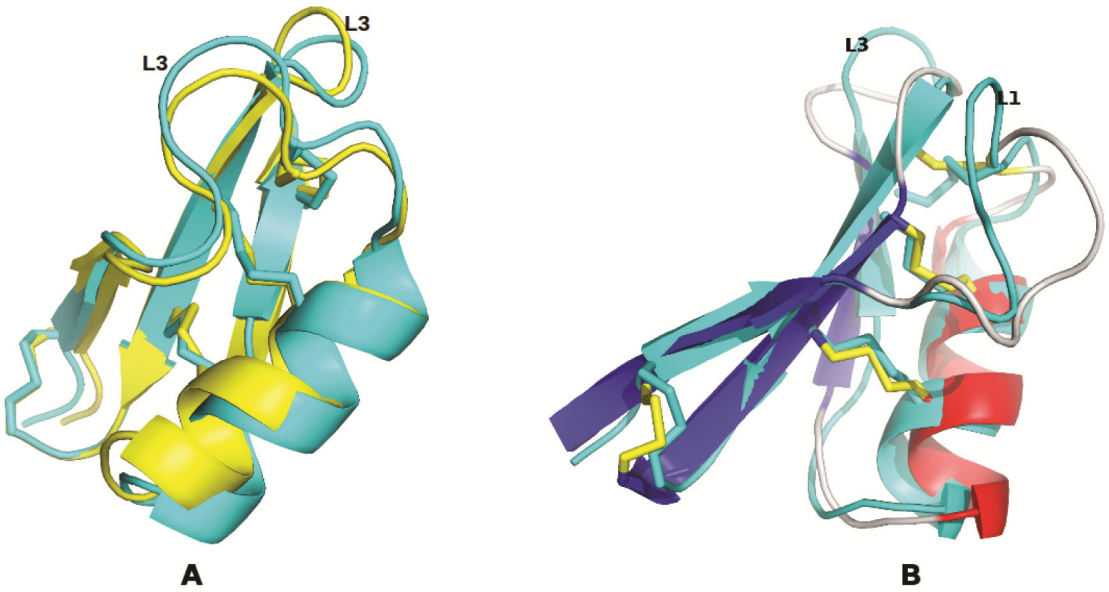
Suppl. Fig. 1 —(A) The plots for root mean square deviation (RMSD in nm) for backbone Cα atomscorresponding to all studied defensin systems in water. (B)The Secondary structure elements givenforeachdefensin *viz.* BcDef, NaD1,2LR3, TPP3 and2N2R fromtopto bottom



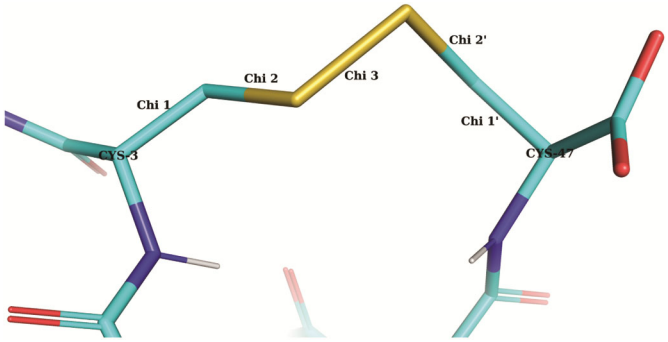
Suppl. Fig. 2 —Totalenergies (inkJ/mol) for all studied defensin systems studied for 10ns with MD simulations in water



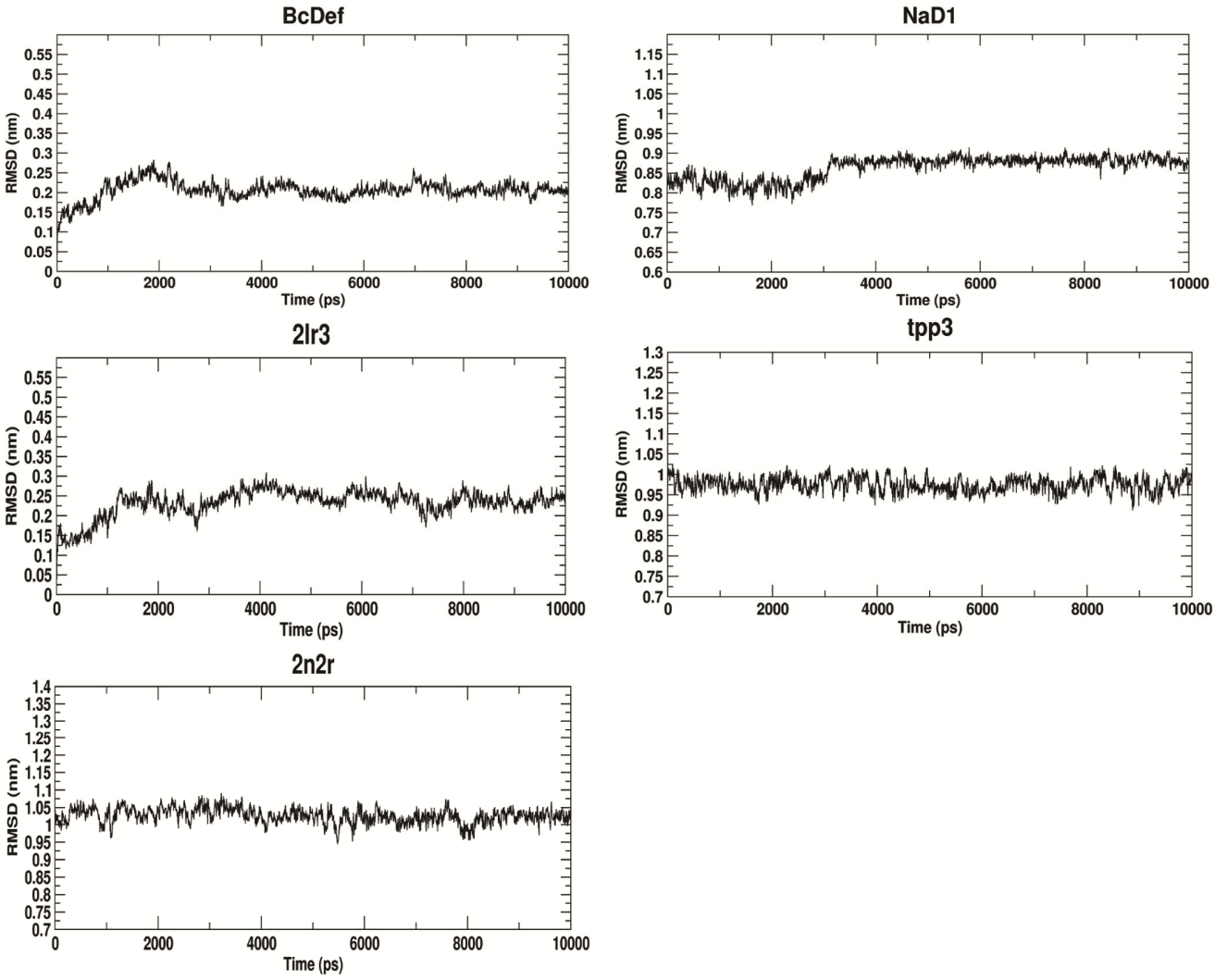
Suppl. Fig. 3 —The plots for radius of gyration (RG) in nm for studied defensins in water. The vectors'xyz' have also been shown and their analysis shows that the values remain within 2 nm from eachvector direction. It means that the structures are stable after certain time. The least fluctuations have been found for tpp3 defensin



Suppl. Fig. 4 —The superimposed structures of BcDef1, starting structure (homology model) with representative structure (cyan) obtained from FEL calculation.(A) cartoon diagramsofrep-3005ps (cyan), rep-3745ps (yellow), the rmsd difference is 1.602 Å;and (B) The structure overlaps for the starting and representative conformation is 1.931Å



Suppl. Fig. 5 —The nomenclature of dihedrals considered for disulfide bond types



Suppl. Fig. 6 — The root mean square deviation (RMSD) for Cα atoms of the defensin peptides and the RMSD values are found to be stable after 3ns of simulation time. The criteria was used to be assured about the quality of MD simulations in water