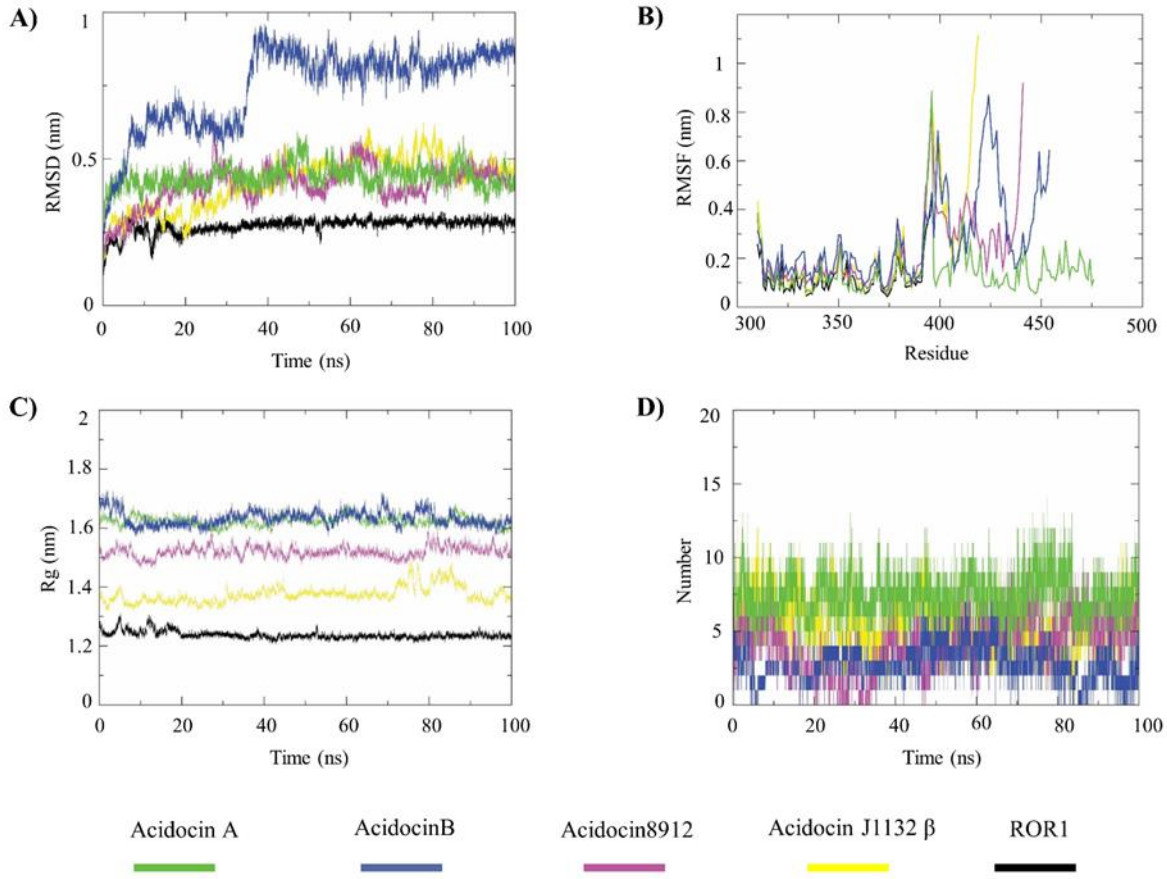


***Figure S1.*** *(A) Root Mean Square Deviation (RMSD) analysis over 100 ns of molecular dynamics (MD) simulations for ROR1 and its complexes with Acidocin A, Acidocin B, Acidocin8912, and Acidocin J1132 β. (B) Root Mean Square Fluctuation (RMSF) analysis showing residue-specific flexibility, with higher RMSF values indicating regions of greater flexibility. (C) Radius of Gyration (Rg) analysis reflecting the compactness of the protein complexes over time. (D) Number of hydrogen bonds formed during the simulation.*

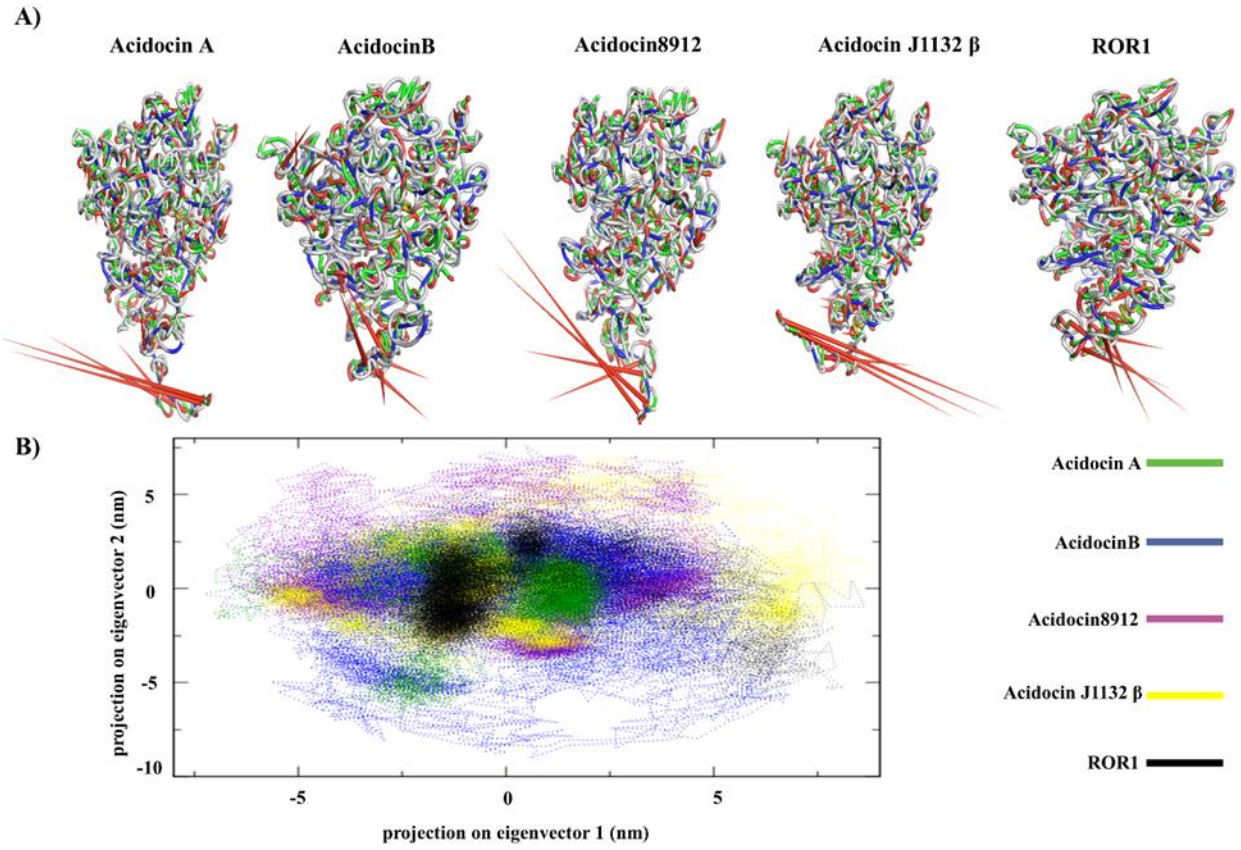


***Figure S2.*** *(A) Porcupine plots illustrating the direction and magnitude of the principal motions identified by PCA for ROR1 and its complexes with Acidocin A, Acidocin B, Acidocin8912, and Acidocin J1132 β. The length and direction of the arrows indicate the extent and orientation of the conformational changes, (B) Projection of the MD simulation trajectories onto the first two principal components (PC1 and PC2) for the ROR1-peptide complexes.*

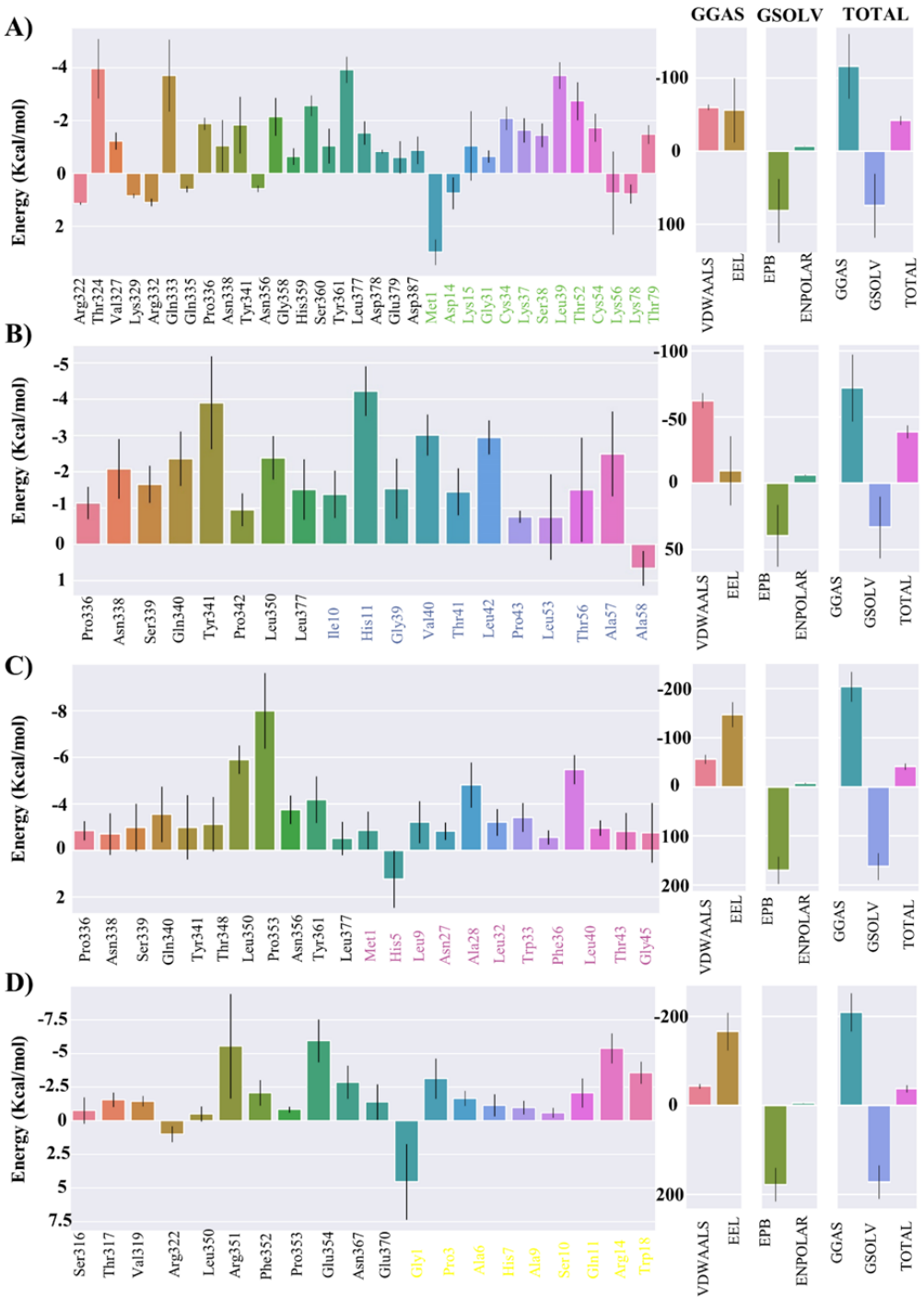


***Figure S3.*** *MM-PBSA binding free energy analysis for ROR1 complexes with (A) Acidocin A, (B) Acidocin B, (C) Acidocin8912, and (D) Acidocin J1132 β. The bar plots on the left depict the contributions of key residues to the binding energy, highlighting significant interactions within each complex. The total binding free energy (ΔTOTAL) shows that Acidocin A has the highest binding affinity, followed by Acidocin8912, Acidocin B, and Acidocin J1132 β, as reflected in the total energy contributions displayed on the right.*

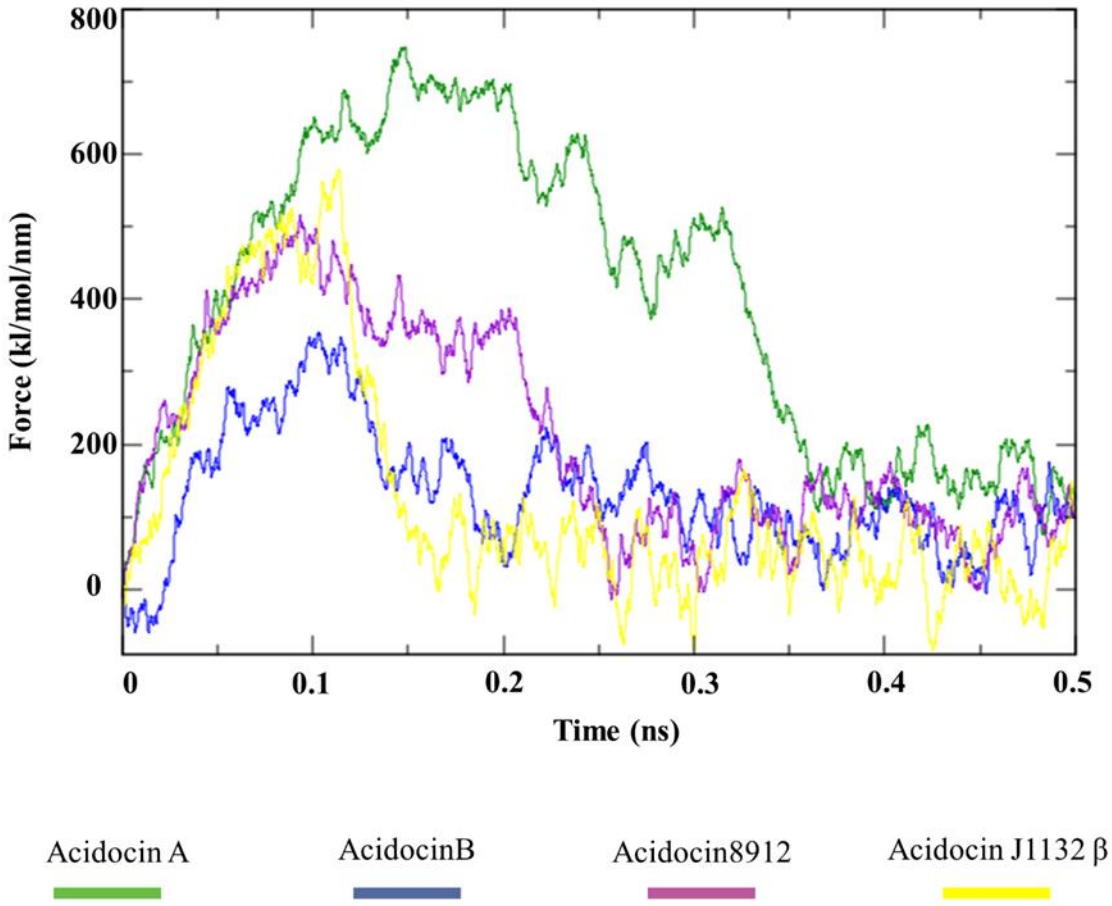


***Figure S4.*** *Force-time graph from Steered Molecular Dynamics (SMD) simulations for the ROR1 complexes with Acidocin A, Acidocin B, Acidocin8912, and Acidocin J1132 β. The graph illustrates the resistance each complex offers during the pulling process, which is indicative of their binding strength and stability.*

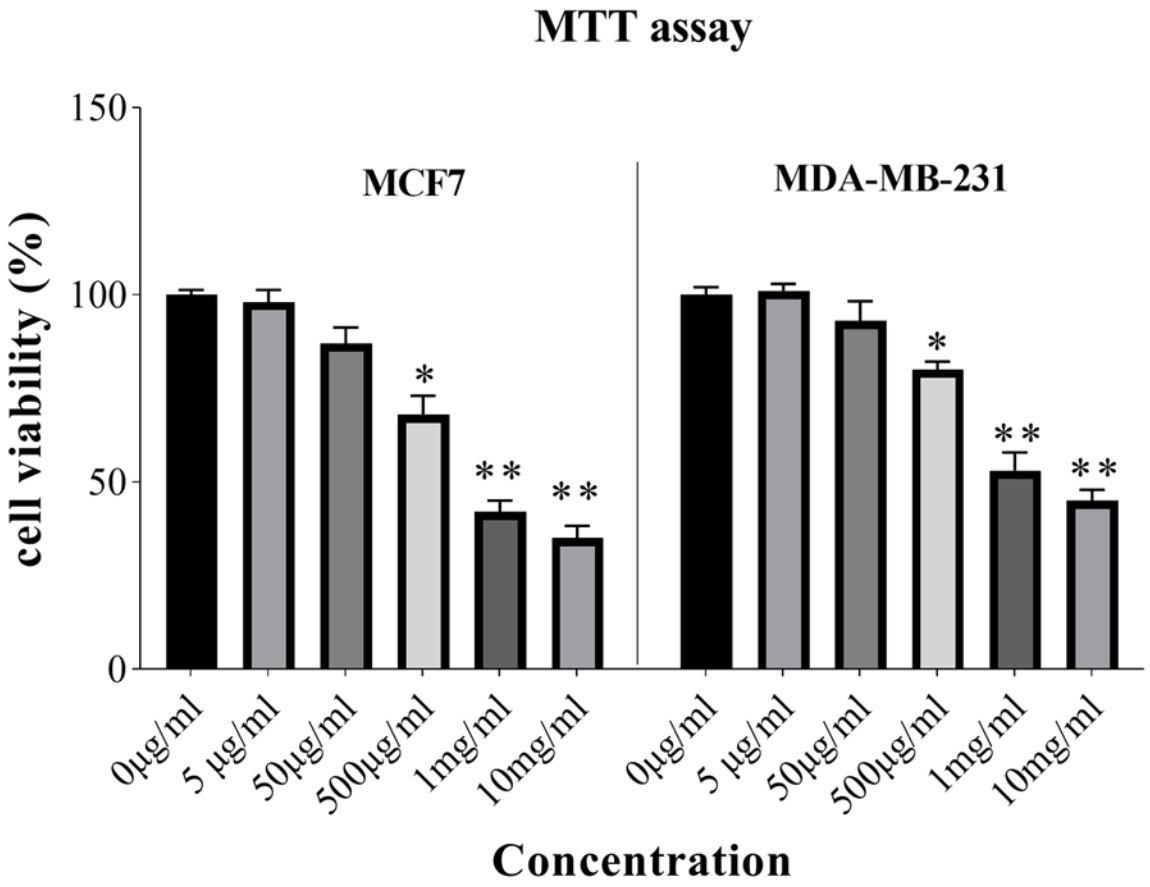


***Figure S5****. Acidocins displays cytotoxic impact in breast cancer cell lines (MCF7 and MDA-MB-231). Viability was assessed in treated cells with crude Acidocin using MTT assay. Results were manifested as mean ± SD and *p < 0.05, **p < 0.01, considered as significant*

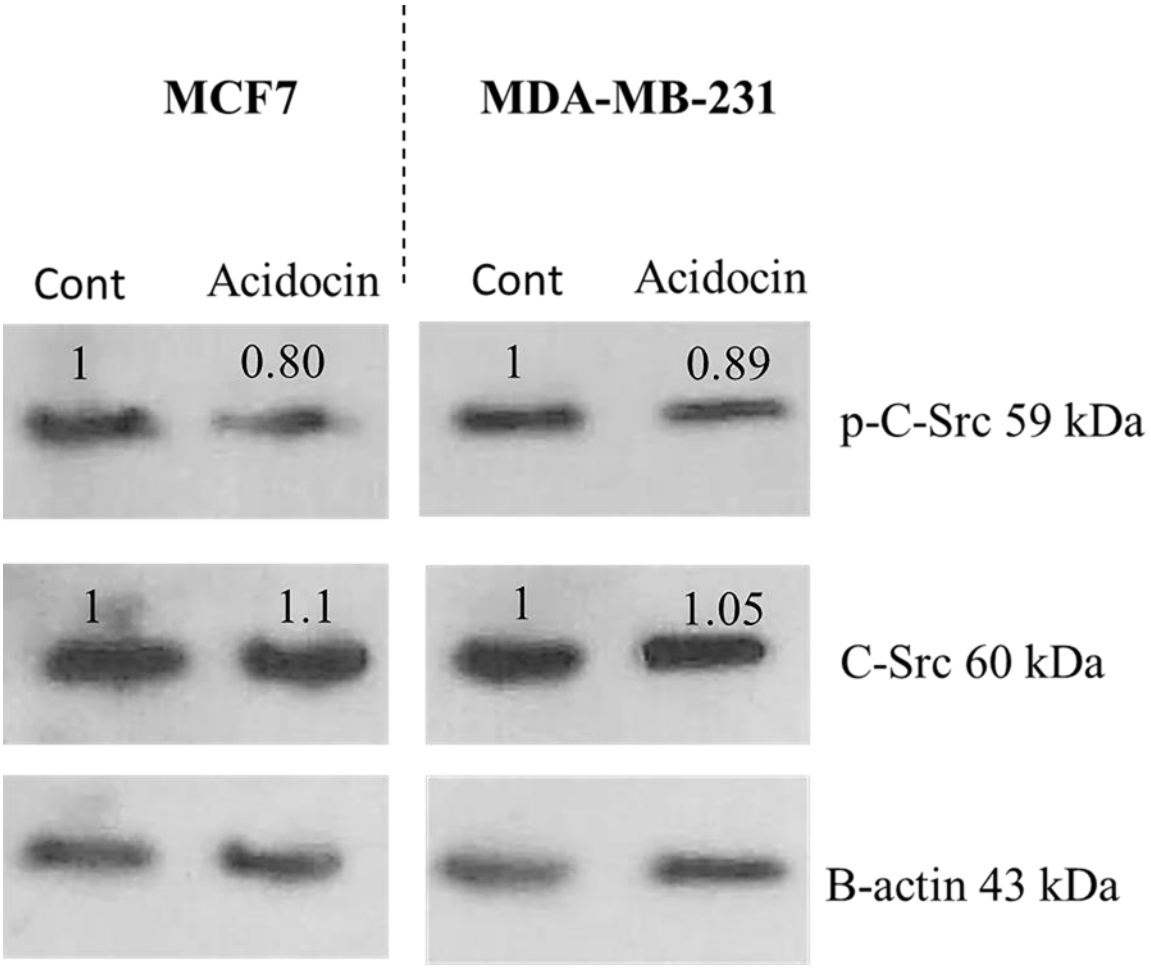


***Figure S6.*** *blockage of ROR1 with crude Acidocin (867 µg/ml and 1mg/ml) in breast cancer cell lines (MCF7 and MDA-MB-231) and its effect on Src phosphorylated level using Western blot assay. Beta-actin was used as normalization*