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Computational interaction study of Human Angiotensin Converting Enzyme with anticancer and antimicobial peptides in diabetic nephropathy

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Objectives: The Diabetic kidney disease (DKD is associated with Diabetic nephropathy (DN) which is the syndrome, represented symptomatically by altered albumin level, lowering glomerular filtration rate etc. leading the kidney failure. The renin-angiotensin system (RAS) has been reported to play the crucial role in the control of kidney function by regulating blood pressure in the body system. Several genes such as ACE, ALR2, APOC1 etc and their genetic variants are majorly affects and associated with Diabetic nephropathy (DN). Several ACE (angiotensin) inhibitors are known but still noted with major challenges of drugs side effect and immunogenecity. This reveals the possibilities to find new drug molecules through performing the *in-silico* interaction study computational interaction/docking and finding and investigate the promiscuity features of antimicrobial and anticancer peptide with exploration of the mechanism of action against 1O8A drug target.

Methods: The structure (Human Angiotensin Converting Enzyme PDB ID : 1O8A) has been downloaded from www.rcsb.org . The blind docking experiment was performed initially with control (C–peptide 3-33 EAEDLQVGQVELGGGPGAGSLQPLALEGSLQ) with target 1O8A, after wards four different Peptides (Aurein 1.2, GLFDIIKKIAESF), pleuricidin 03 GRRKRKWLRRIGKGVKIIGGAALDHL, (pleuricidin 07 (RWGKWFKKATHVGKHVGKAALTAYL) , human neutrophil peptide-1 (HNP-1, ACYCRIPACIAGERRYGTCIYQGALWAFCC) were docked with same target on default parameters on Hpepdock server

Results: The control (C protein has shown docking score -156.601 while the four anticancer and antimicrobial peptides shown comparatively better docking score (Aurein 1.2 (168.371), pleuricidin 03 (-230.588), pleuricidin 07 (-215.952), human neutrophil peptide-1 (-229.749). comparing with control pleuricidin 03 was the best hence selected reveals the binding pattern with histidine and aspartic after Molecular Dynamics simulation results demonstrated the structural stability binding with (histidine 153, Glutamic 188, Arginine 191 etc.).

Conclusions: it is concluded that that pleuricidin 03 peptide shown promiscuity by exhibiting better docking/interaction and could be further extended by wet lab based and more interactions on MD simulation based experiments