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Design, synthesis, molecular docking, molecular characterization and biological activity of novel synthetic peptide derivatives

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Our interest in the design, synthesis and biological investigations of peptides is, progressively, reported. Herein, the search for potent biological agents presented and updated area of the organo-biochemical literature. Herein, Nα-1, 3-benzenedicarbonyl linear peptide candidates, has the structure: Nα-1, 3-benzenedicarbonyl-bis-(Amino acids)-X. On the other hand, Nα-benzenedicarbonyl bridged cyclic-penta-peptides, having the structure: Cyclic-[Nα- benzendicarbonyl- bis-(dipeptide)-L-Lys]-Y. Variable synthetic coupling methods, in solution, as well as experimental reaction conditions, were experimented. The candidates were, chromatographically purified and spectroscopically characterized. A preliminary cytotoxicity evaluation, against eight human cancer cell lines was realized (National Cancer Institute, Egypt). The detailed cytotoxic and hepatotoxic results, compared to those of five common anticancer drugs and their biochemical assays particularly, as histone deacetylase inhibitors, are currently in progress. Structure activity relationships were outlined and suggested prospective were proposed.