**Figure S1**. Ten clusters of 3D structures of **(A)** Tat(49-57)-NH$_2$ and **(B)** PTD4 peptides in water and of **(C)** Tat(49-57)-NH$_2$ and **(D)** PTD4 peptides 30 % (v/v) TFE, respectively. Each cluster is represented by one structure. All structural models were generated using the AMBER program.