Electronic supplementary information (ESI)

Factors influencing the catalytic activity of metal-dependent histidine-rich peptides: sequence, conformation, stereochemistry, self-assembly or their interplay?

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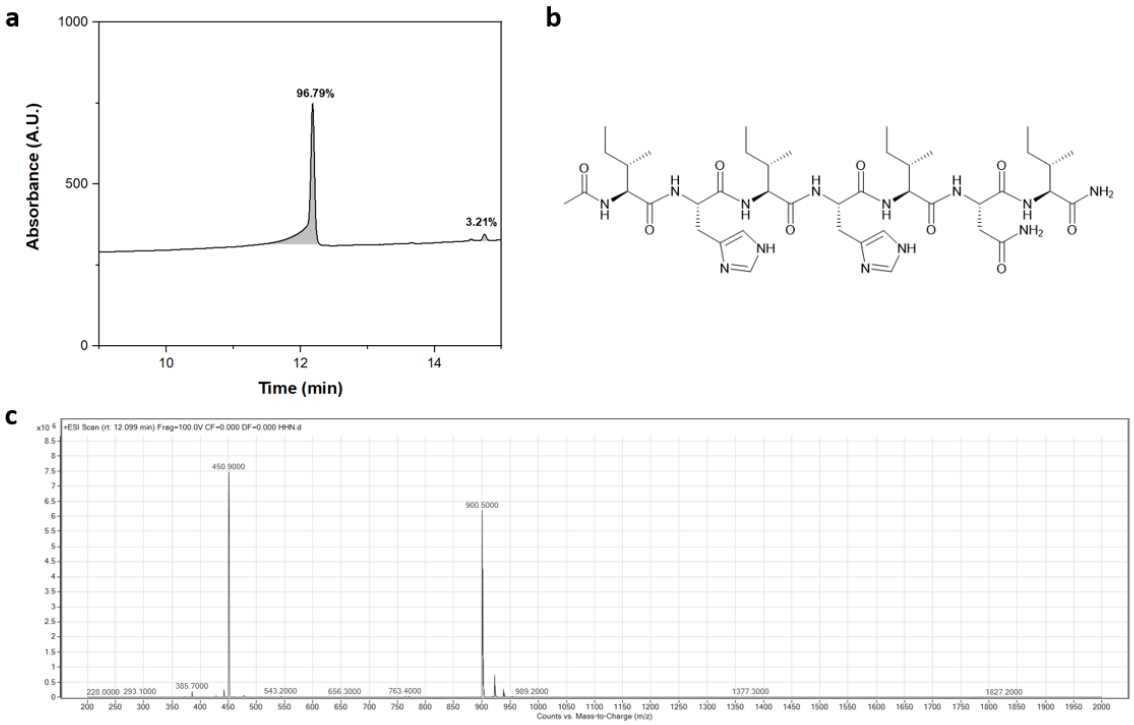

Figure S1: **a**) LC chromatogram at 220 nm (purity of 96.79%), **b**) chemical structure and (**c**) the MS trace for Ac-IHIHINI-Am (peptide A) (m/z 900.5) .

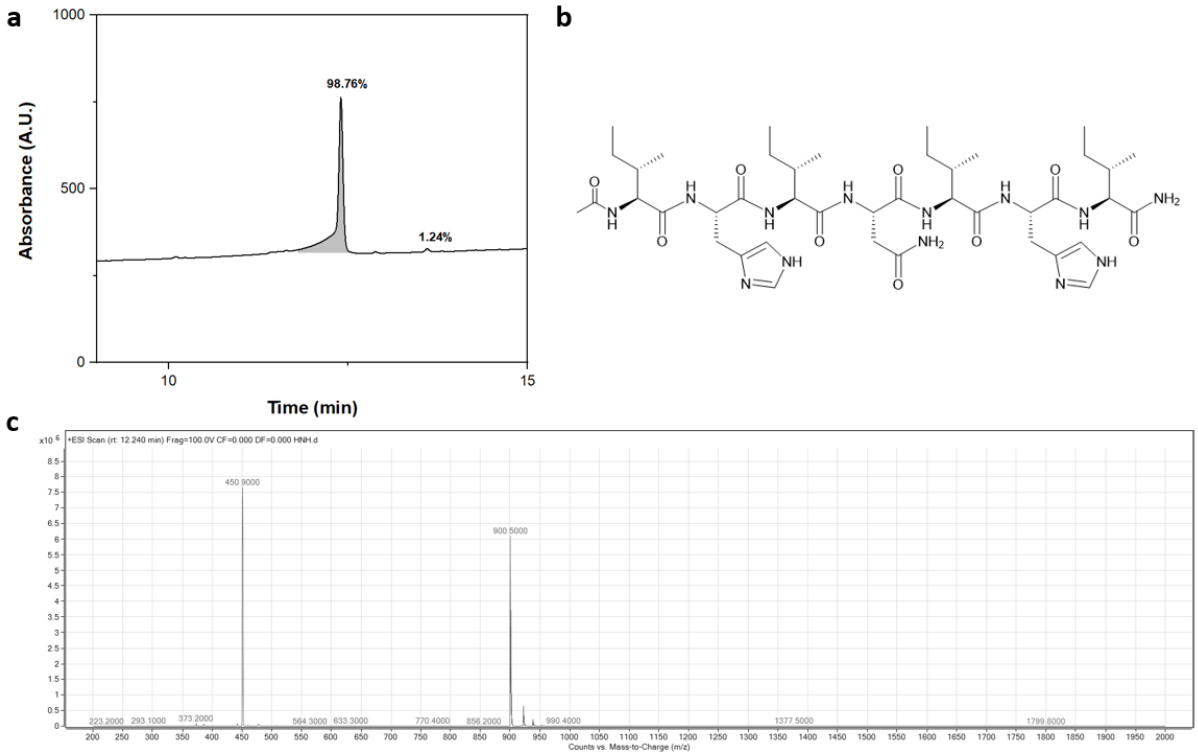

Figure S2: **a**) LC chromatogram at 220 nm (purity of 98.76%), **b**) chemical structure and (**c**) the MS trace for Ac-IHINIHI-Am (peptide B) (m/z 900.5) .

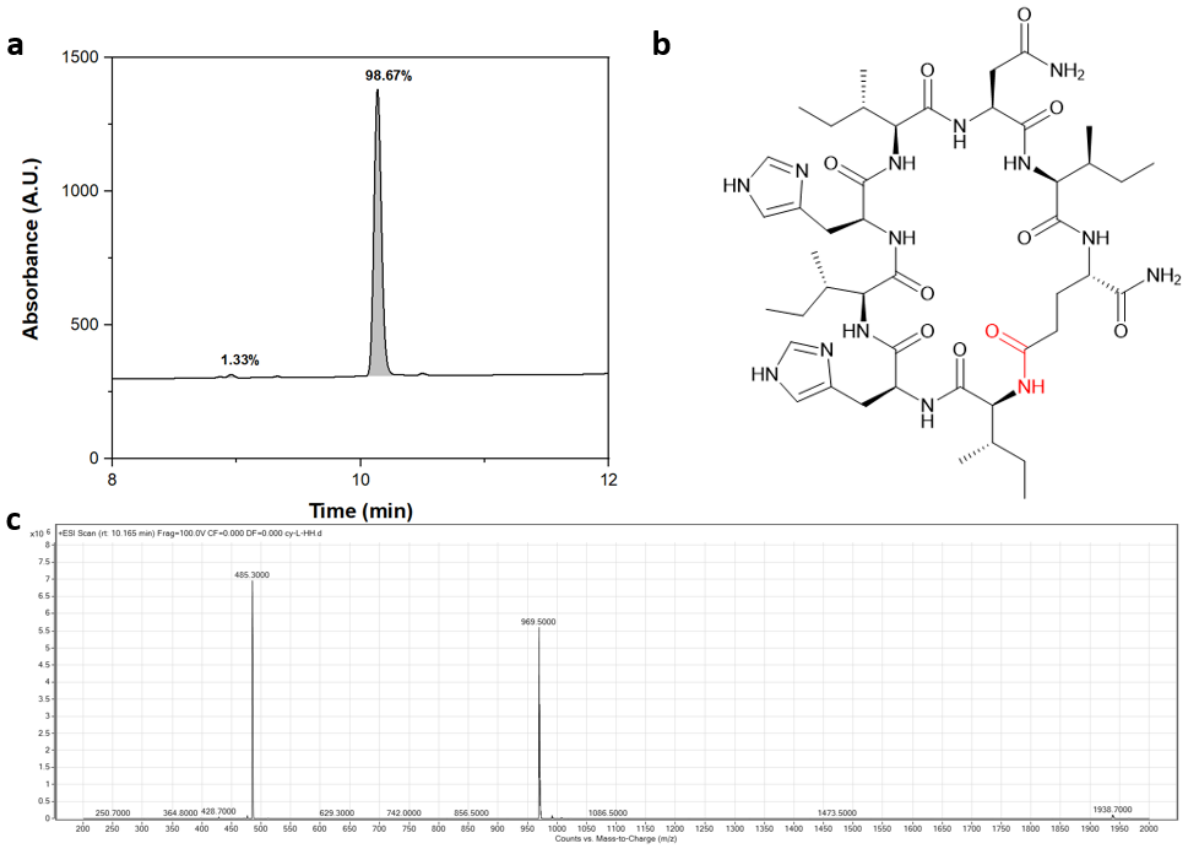

Figure S3: **a**) LC chromatogram at 220 nm (purity of 98.67%), **b**) chemical structure and (**c**) the MS trace for [IHIHINI]-Am (cy-HH) (m/z 969.5) .

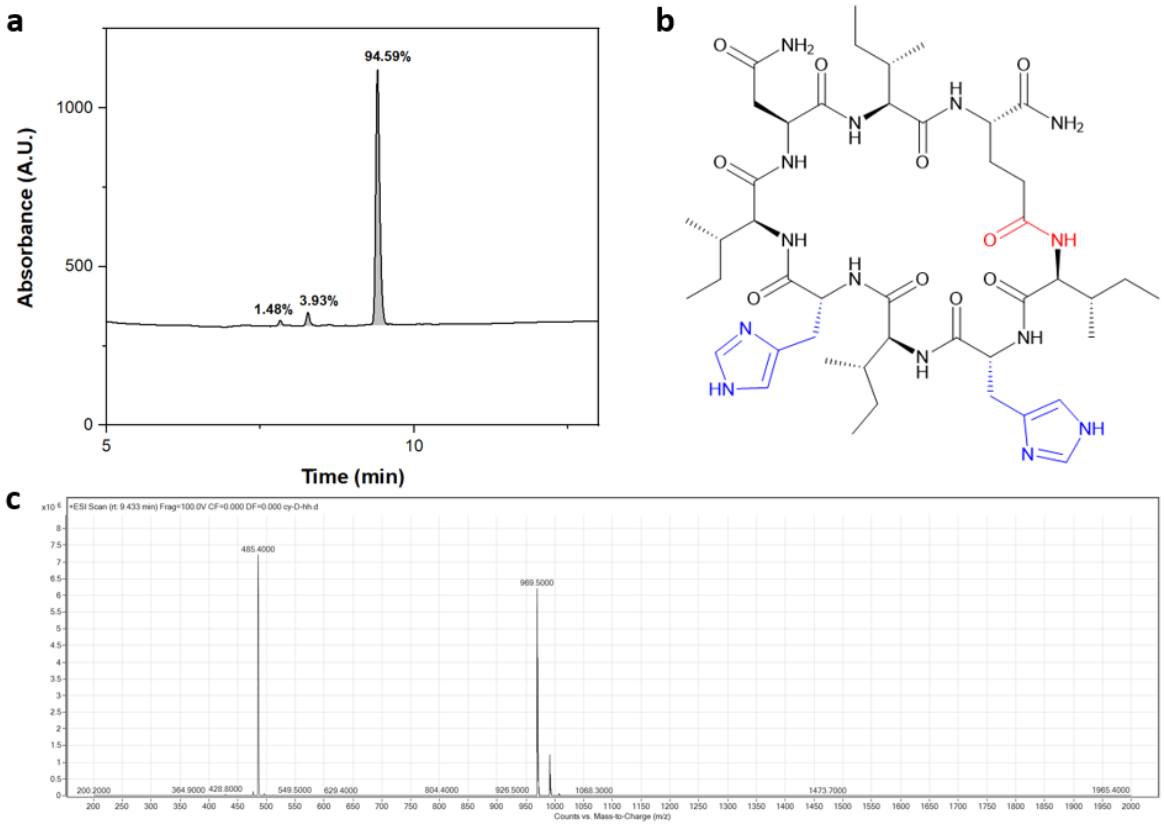

Figure S4: **a**) LC chromatogram at 220 nm (purity of 94.59%), **b**) chemical structure and (**c**) the MS trace for [IhIhINI]-Am (cy-hh) (m/z 969.5) .

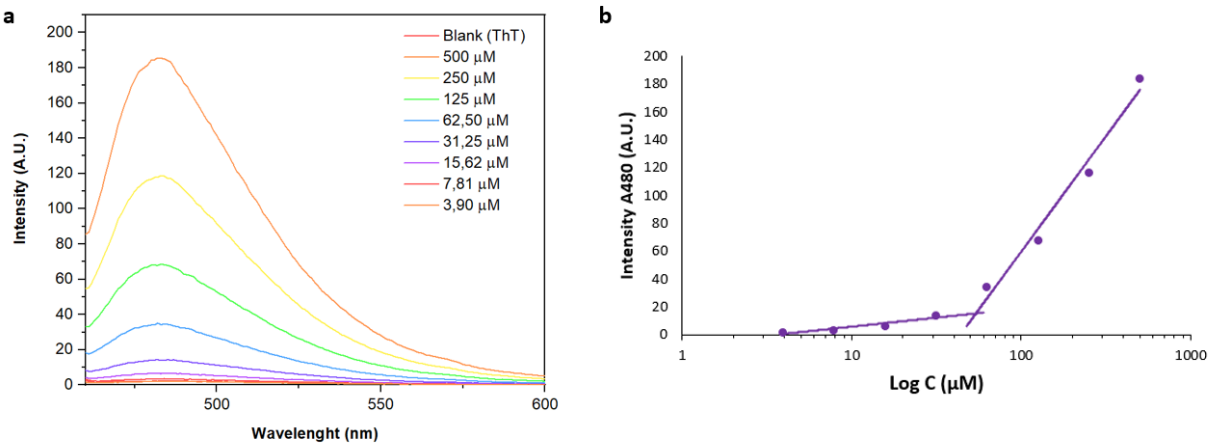

Figure S5: **a**) Fluorescence intensities of ThT at different concentrations of cy-hh, **b**) CAC in MiliQ water, plotted as a function of ThT fluorescence emission at 480 nm.

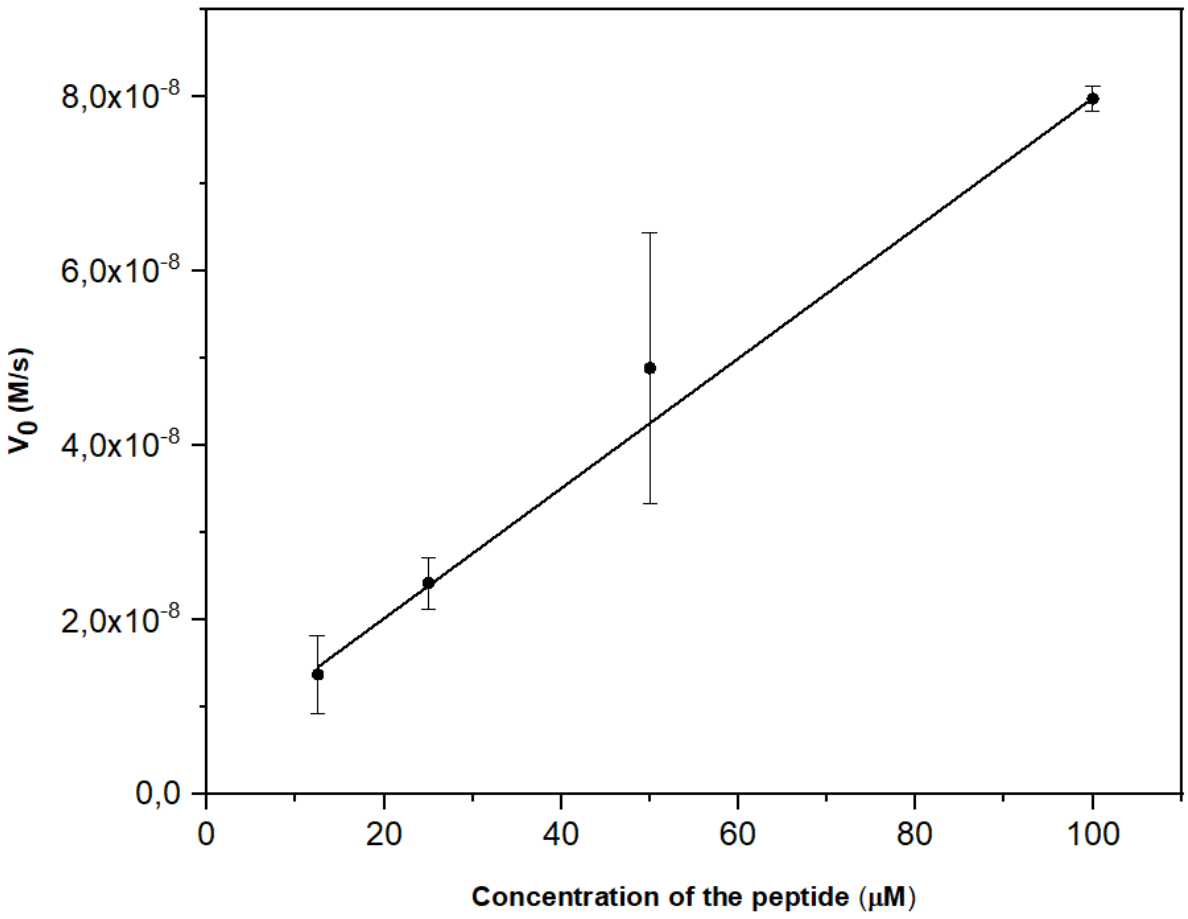

Figure S6: Dependence of p-NPA hydrolysis rate on the concentration of the peptide B.

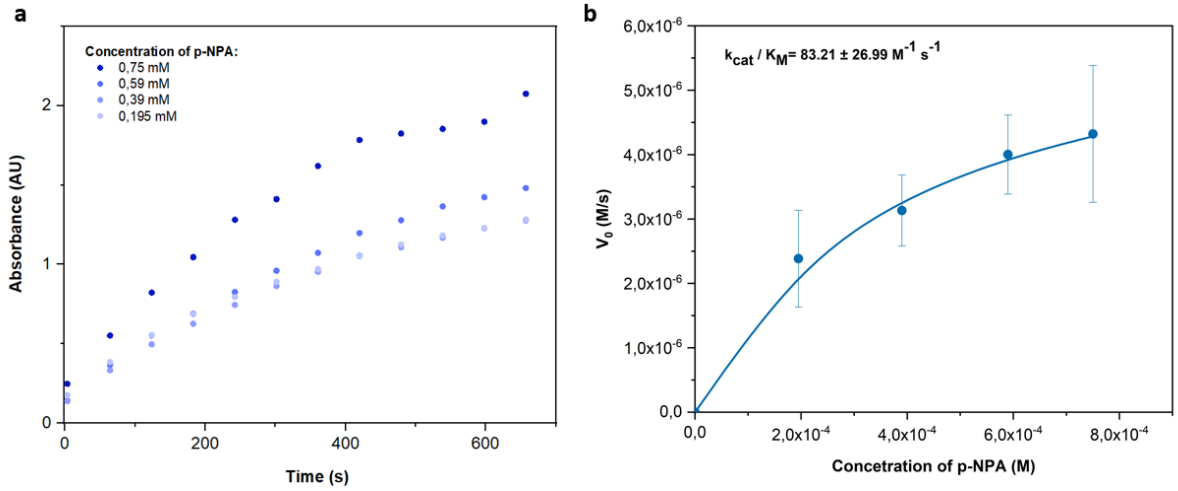

Figure S7: (a) Kinetic plot and (b) Michaelis-Menten graph for peptide A in 25 mM TRIS, 1 mM $ZnCl_2$ at pH 8 was employed for the determination of a k_{cat}/K_M value of 83.21 ± 26.99 M^{-1} s^{-1}.

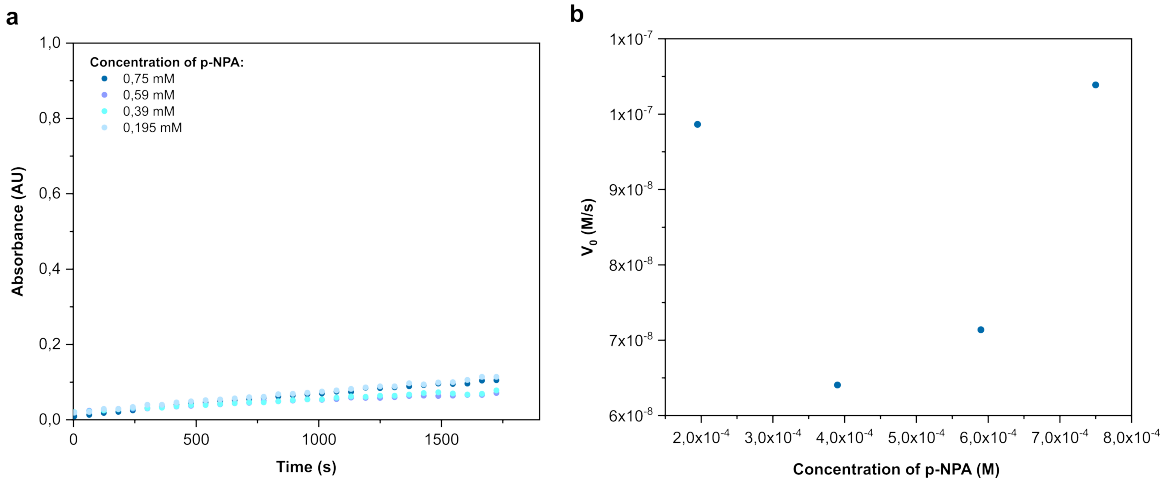

Figure S8: (a) Kinetic plot and (b) Michaelis-Menten graph for Peptide A in 25 mM TRIS Buffer at pH 7.4 without $ZnCl_2$, demonstrating minimal catalytic activity resulting in the inability to calculate kinetic parameters.

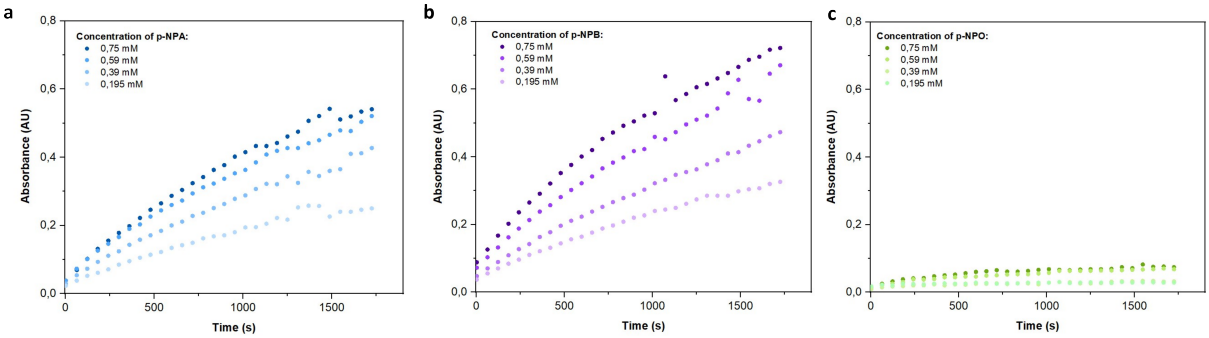

Figure S9: Kinetic plots of a) p-NPA, b) p-NPB, and c) p-NPO assayed for Peptide A at pH 7.4 in 25 mM TRIS Buffer with 1 mM $ZnCl_2$.

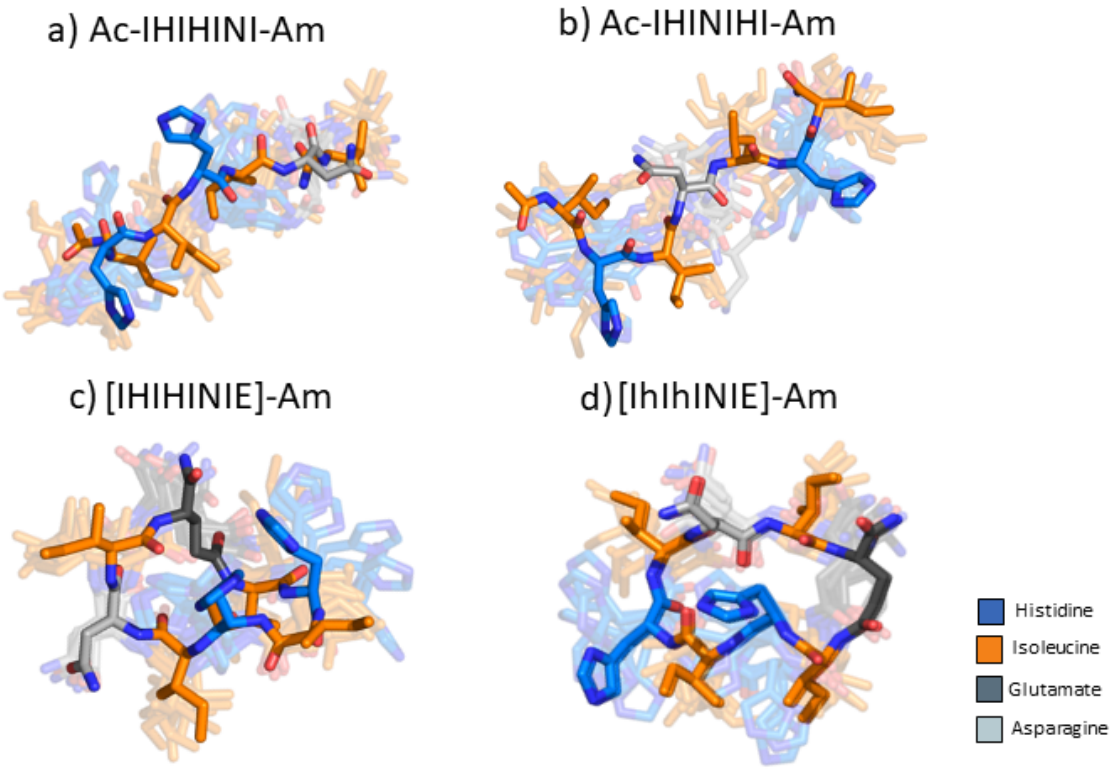

Figure S10: Cluster analysis of (**a**) Ac-IHIHINI-Am; (**b**) Ac-IHINIHI-Am; (**c**) [IHIHINIE]-Am; (**d**) [IhIhINIE]-Am. Clusters 1 to 10 are overlapped, the most dominant cluster is opaque, the remaining 9 are transparent.

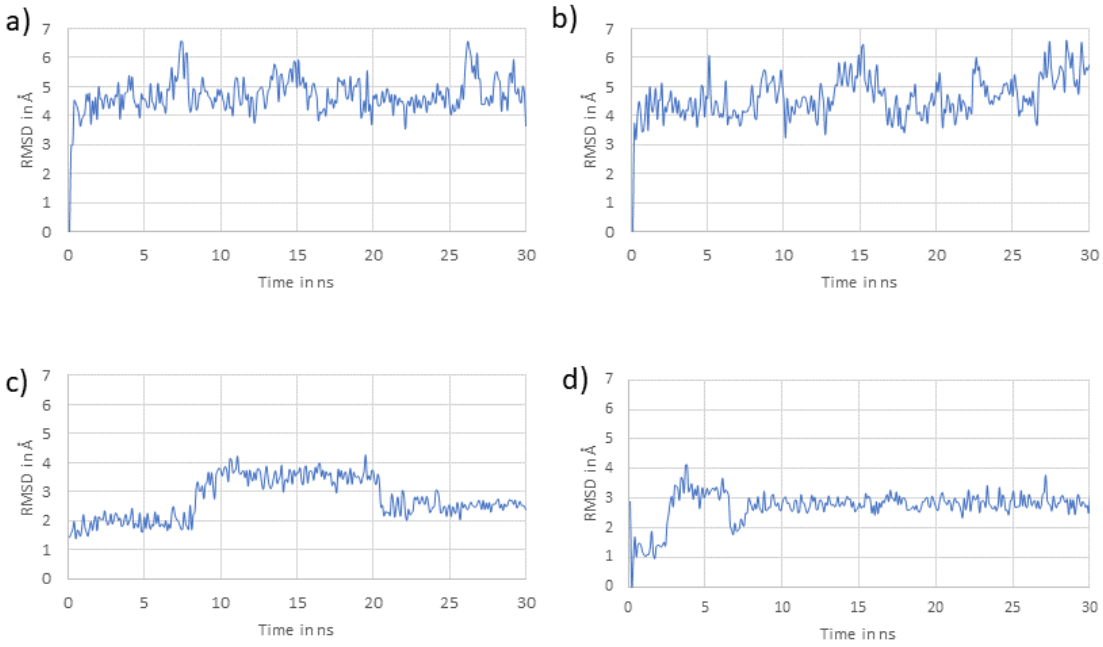

Figure S11: RMSD plots for (**a**) Ac-IHIHINI-Am; (**b**) Ac-IHINIHI-Am; (**c**) [IHIHINIE]-Am; (**d**) [IhIhINIE]-Am.

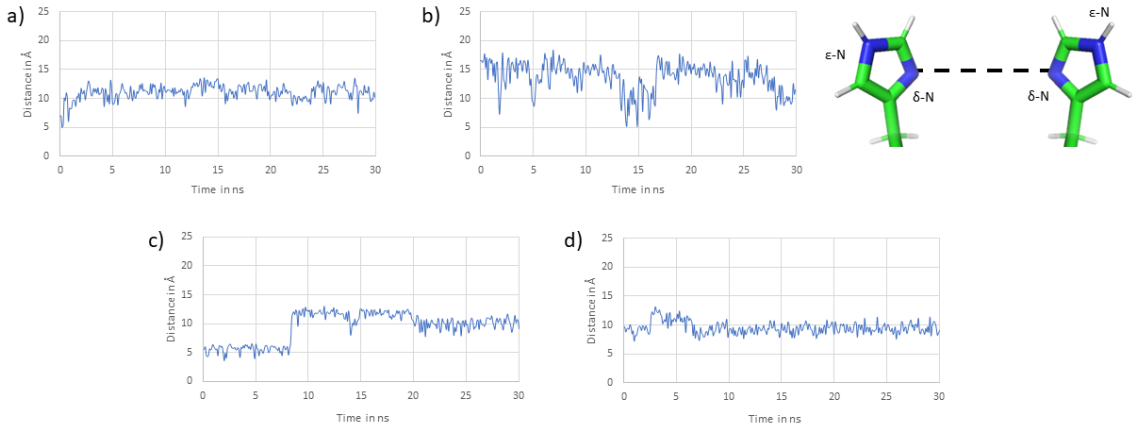

Figure S12: N-δ-His to N-δ-His average distance plots (reported in Table 3) for (**a**) Ac-IHIHINI-Am; (**b**) Ac-IHINIHI-Am; (**c**) [IHIHINIE]-Am; (**d**) [IhIhINIE]-Am.

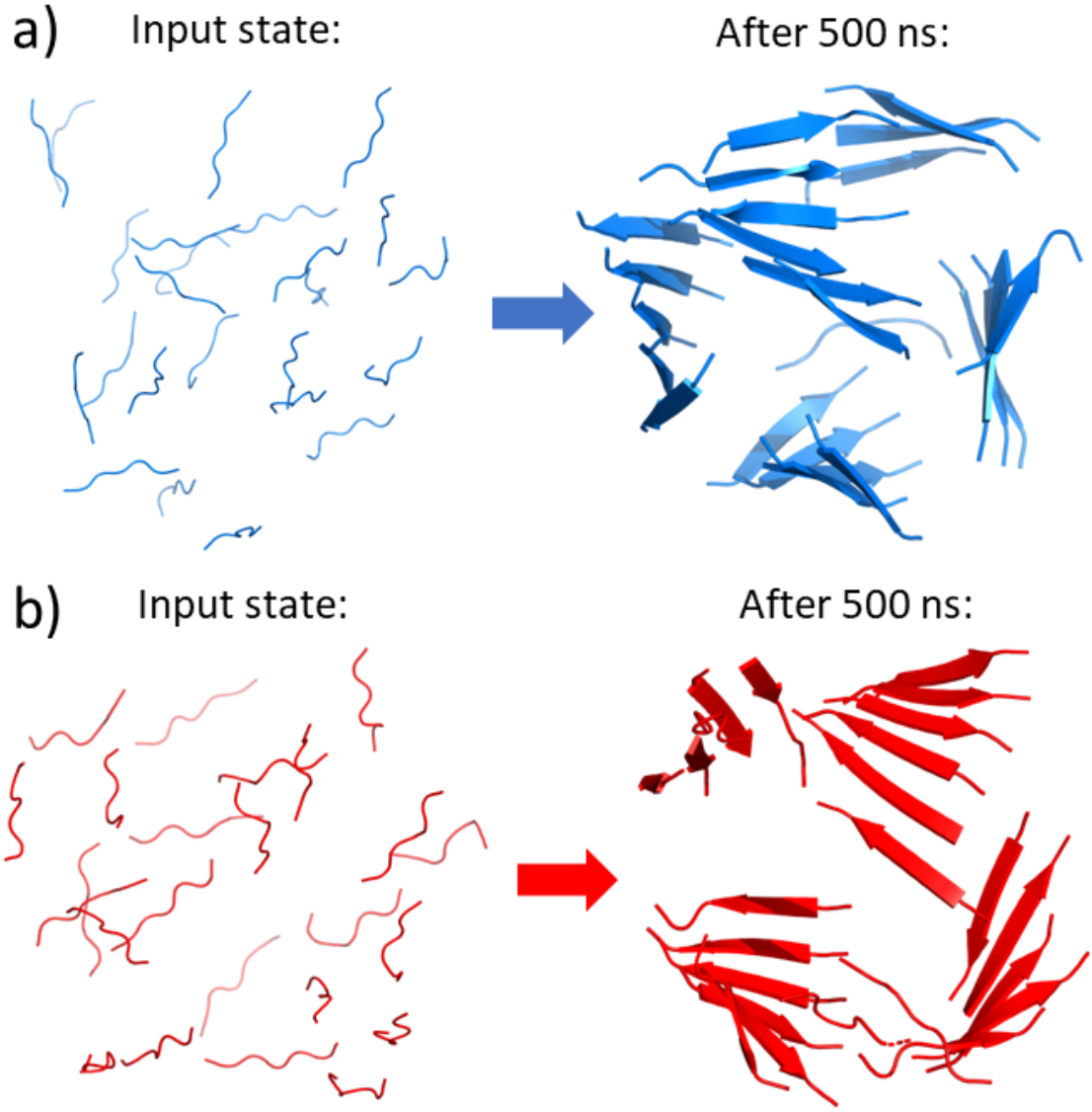

Figure S13: MD simulations of linear peptides (**a**) Ac-IHIHINI-Am; (**b**) Ac-IHINIHI-Am. The images show the initial Monte-Carlo placement of 24 peptides in solution and their aggregation into β-sheet structures after 500 ns.

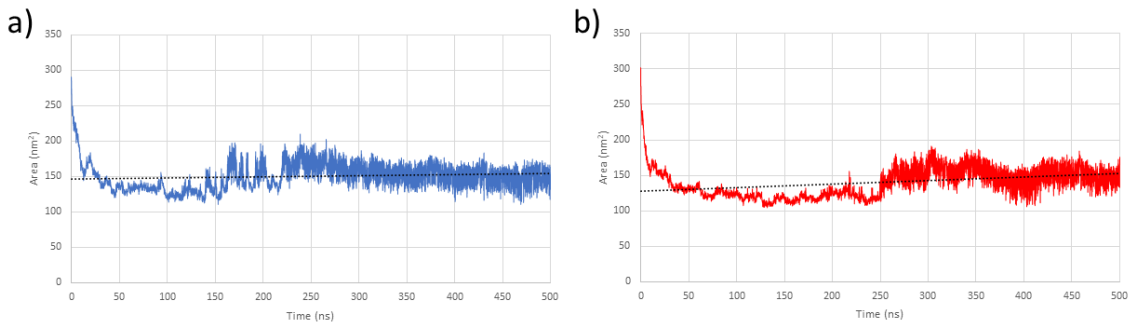

Figure S14: SASA analysis of (**a**) Ac-IHIHINI-Am; (**b**) Ac-IHINIHI-Am simulations in water and 0.08 M Tris buffer