Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supporting information for: Graph-based analyses of H-bond networks and unsupervised learning reveal conformational coupling in prion peptide segments

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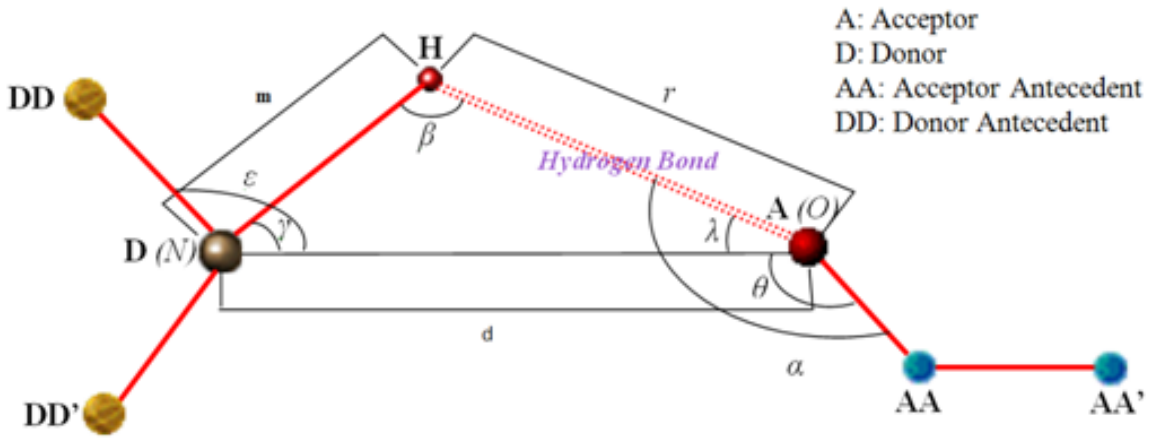

Figure S1: Hydrogen-bond geometric definition criteria. H-bond is formed when: $r \leq 0.25nm, \beta \geq 150°$; and when $d \leq 0.35nm, \gamma \leq 35°$.

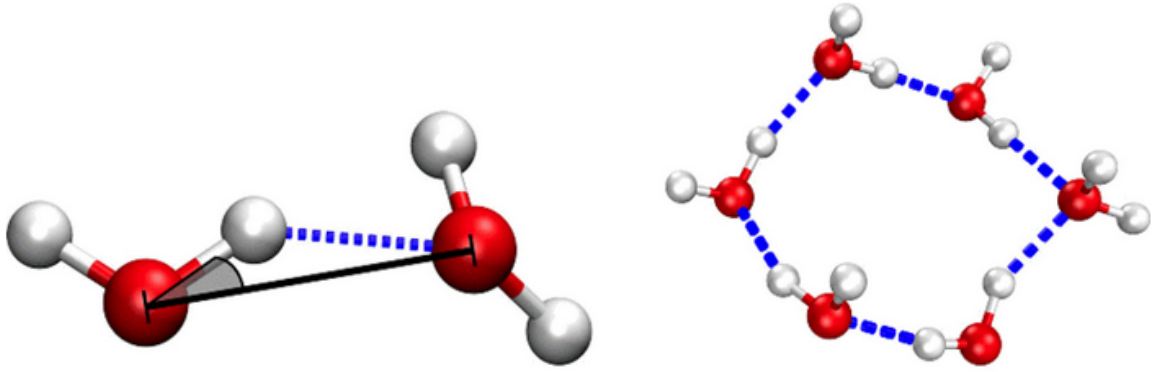

Figure S2: Geometric definition of a hydrogen bond, and a loop of six hydrogen-bonded water molecules.

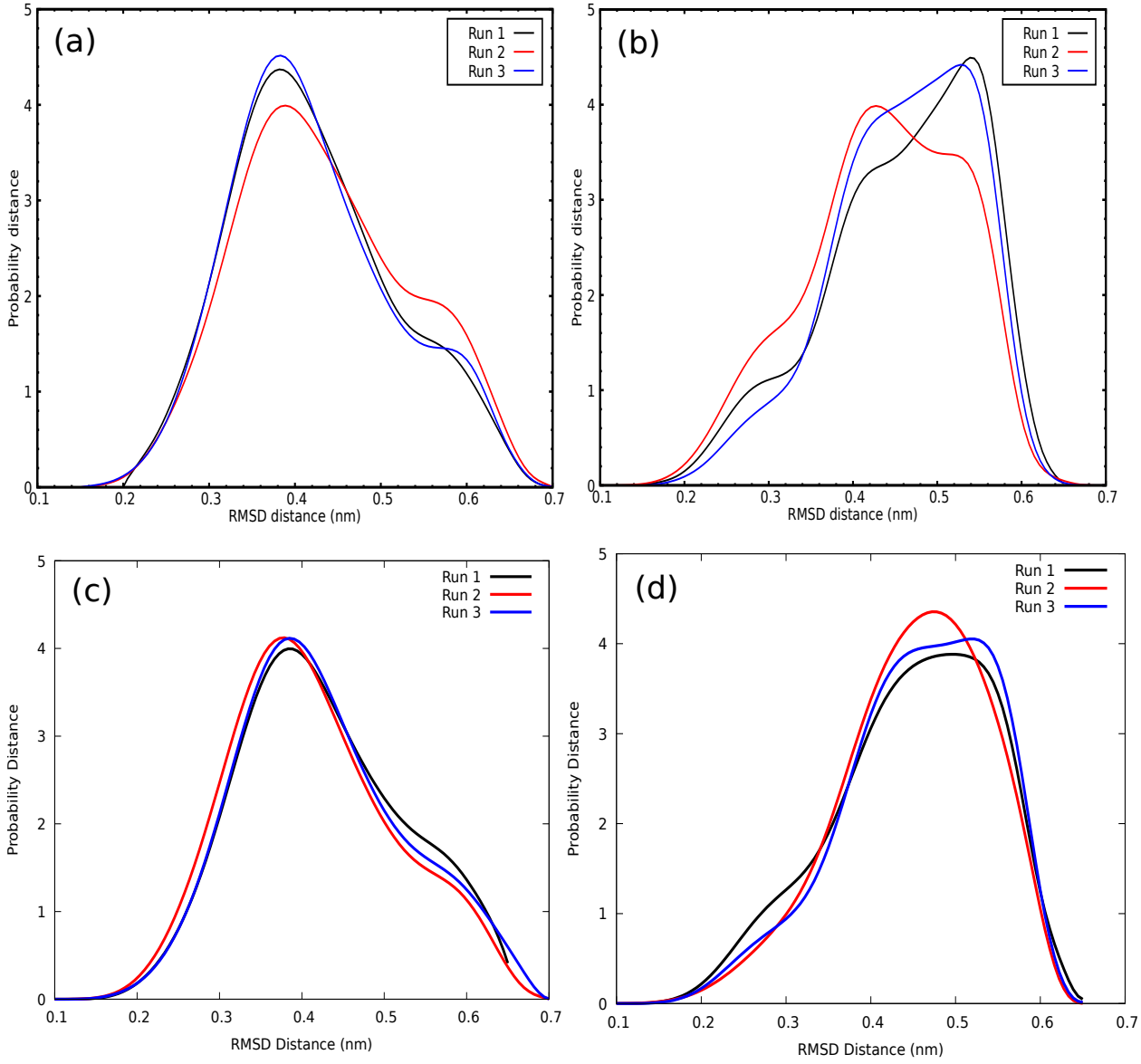

Figure S3: Three independent runs of RMSD probability distribution plots for G127/M129 (a), V127/V129 (b), G127/V129 (c) and V127/M129 (d).

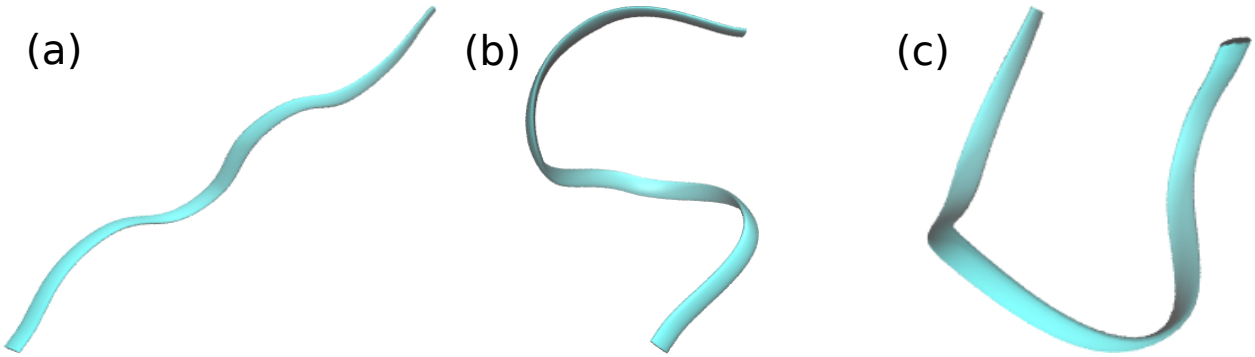

Figure S4: The three dominant clusters found in the four systems. The open or unfolded state is represented by (a), while the partially-folded (or S-shaped conformation) and the folded (or U-shaped conformation) are shown in b and c, respectively.

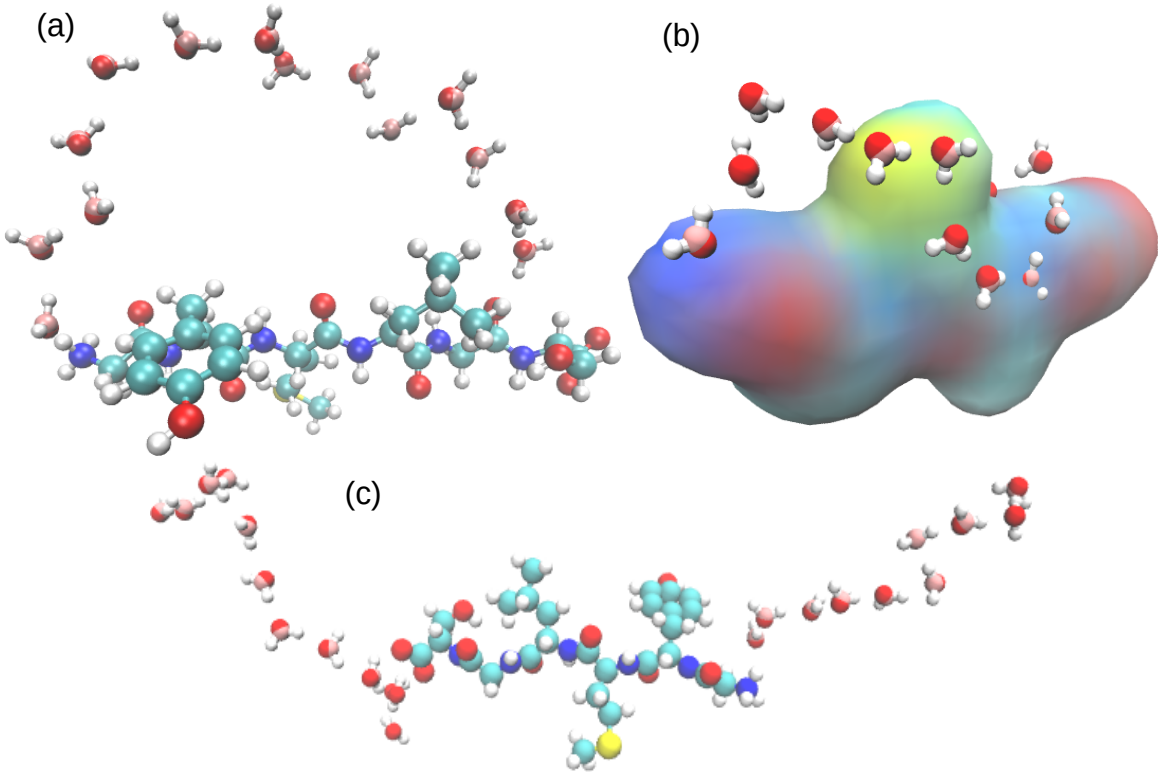

Figure S5: Water wire path lengths around peptides illustrating H-bond networks in the vicinity of peptide structures. The water wire path lengths provide insights into the solvation dynamics and hydrogen bonding patterns involved in peptide-water interactions.

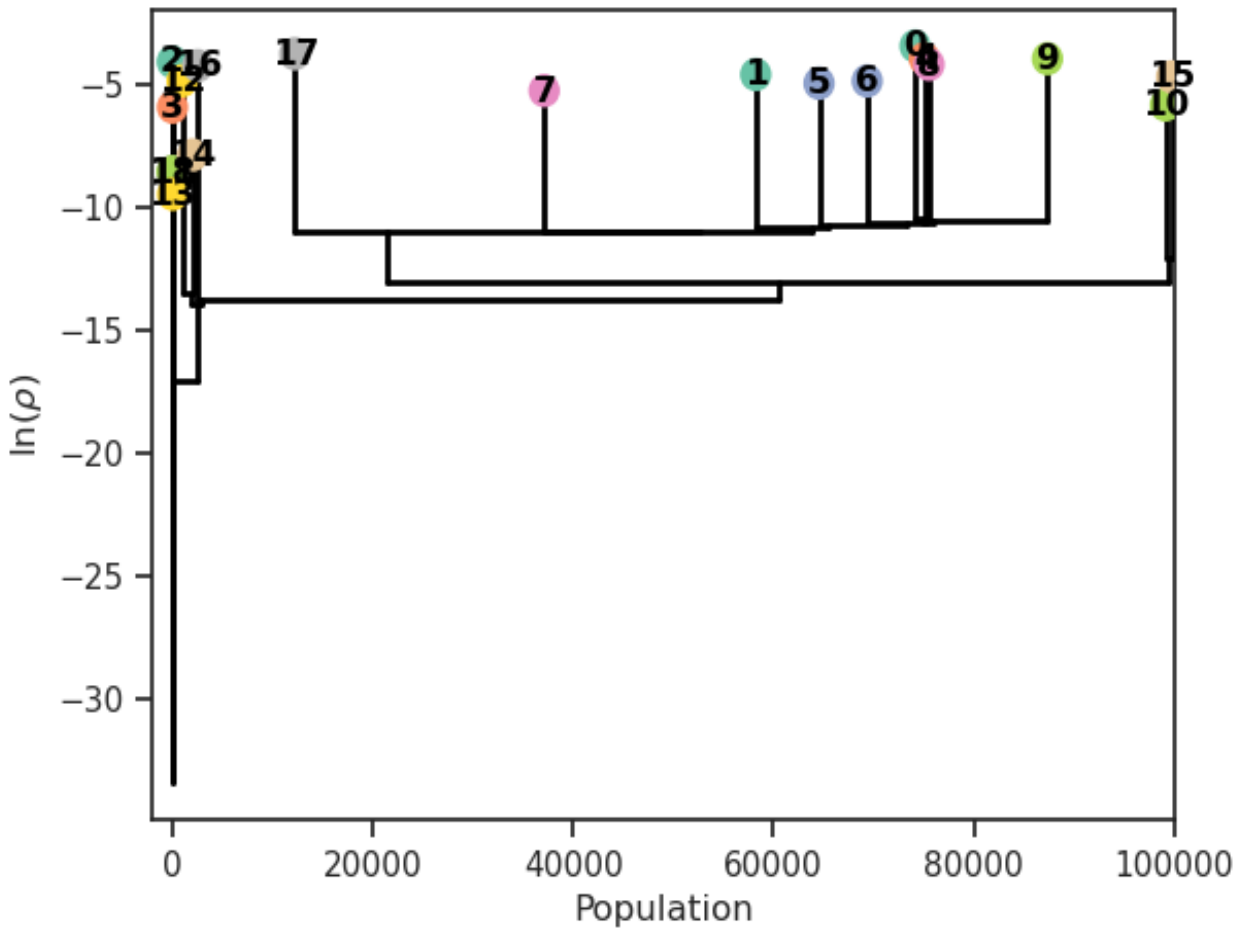

Figure S6: Dendrogram representation illustrating a rough free energy landscape. The various conformations of the cluster center structures are depicted adjacent to their corresponding density peaks.

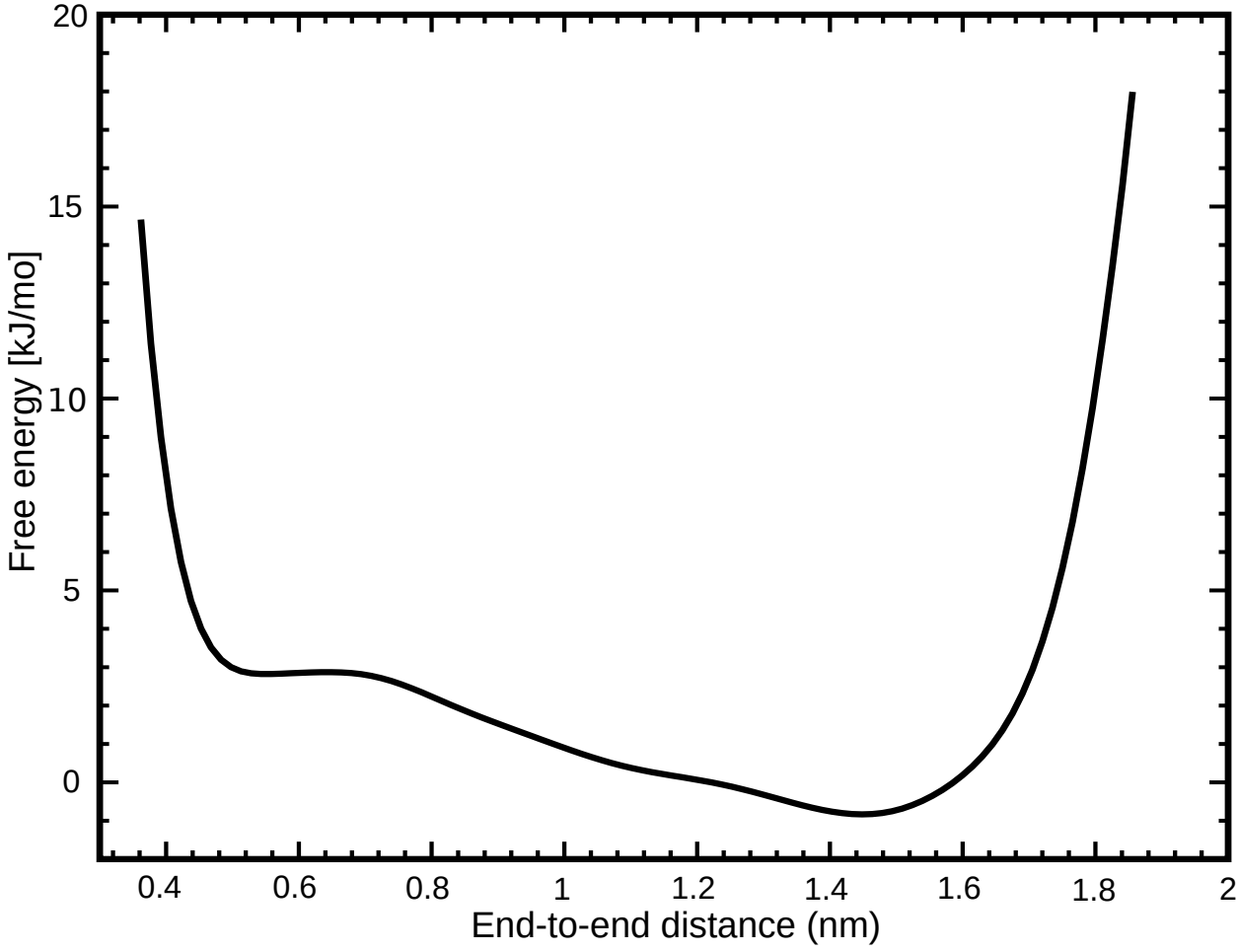

Figure S7: One-dimensional free energy landscape of G127/M129 peptide using end-to -end distance as a collective variable.

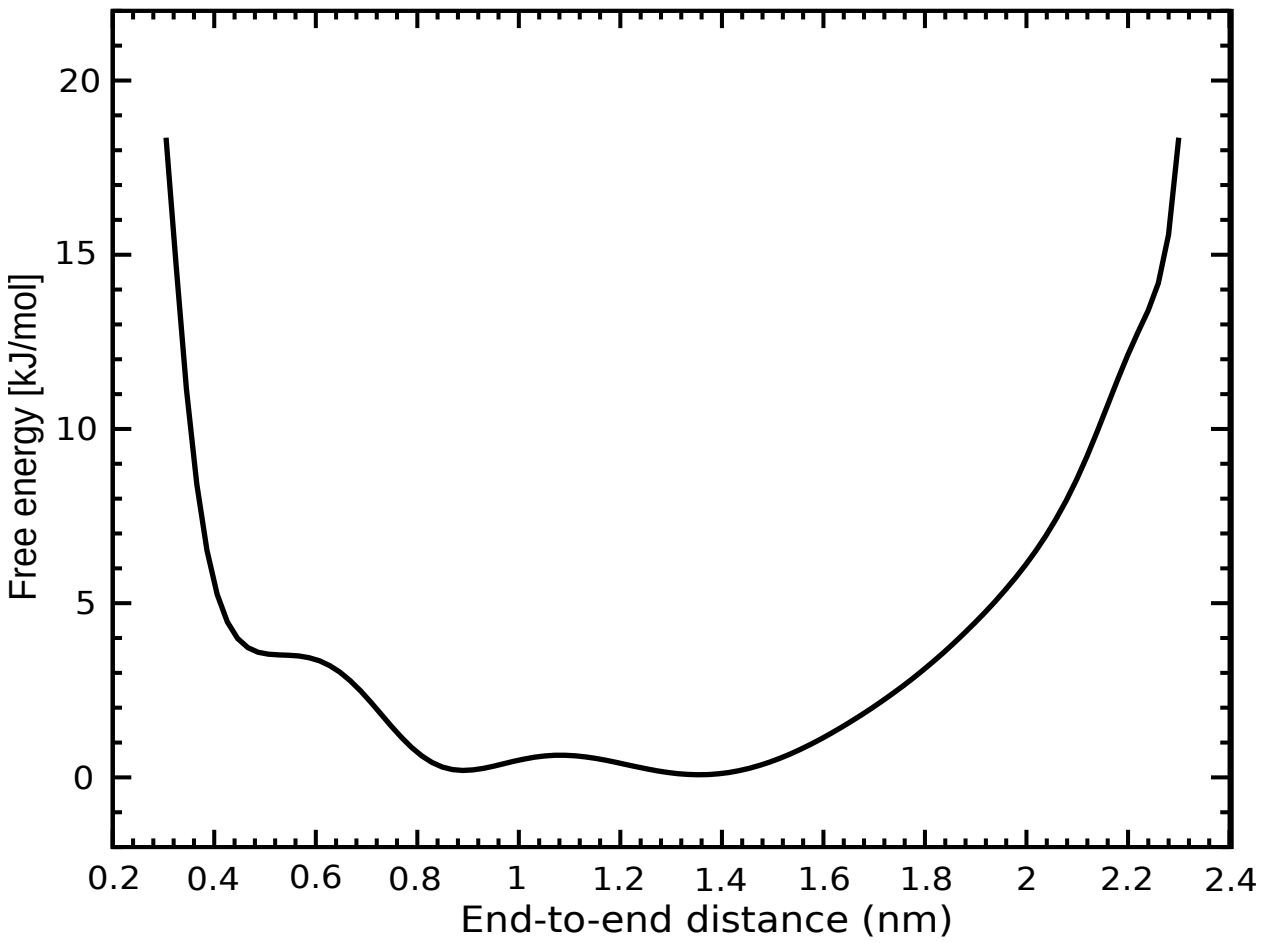

Figure S8: One-dimensional free energy landscape of V127/V129 peptide using end-to -end distance as a collective variable.

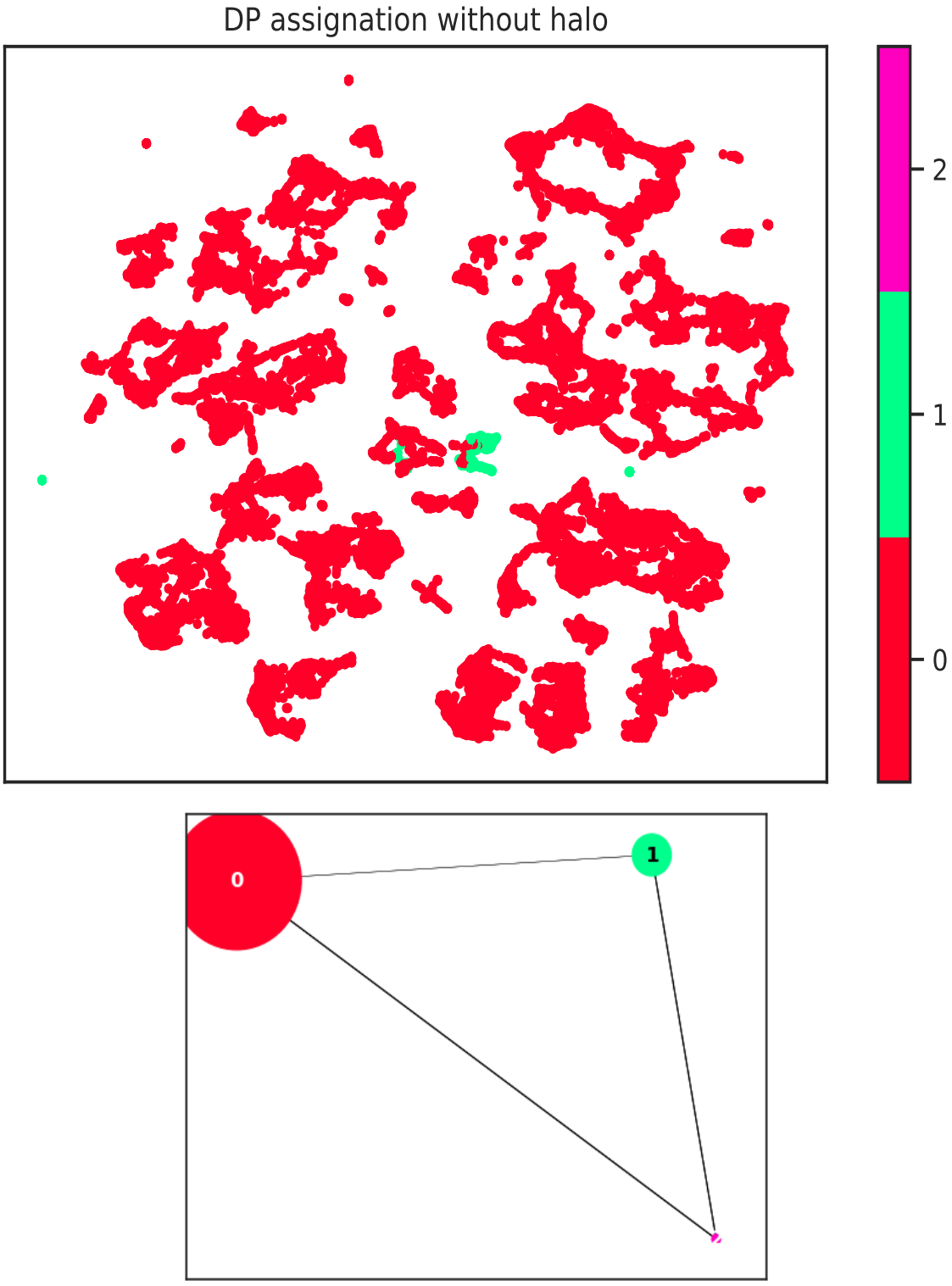

Figure S9: Plot of the DP clustering assignation showing distribution of clusters on a decision graph for G127/MET129 peptide (upper panel), and a 2D multidimensional scaling projection showing similarity relationships among clusters.

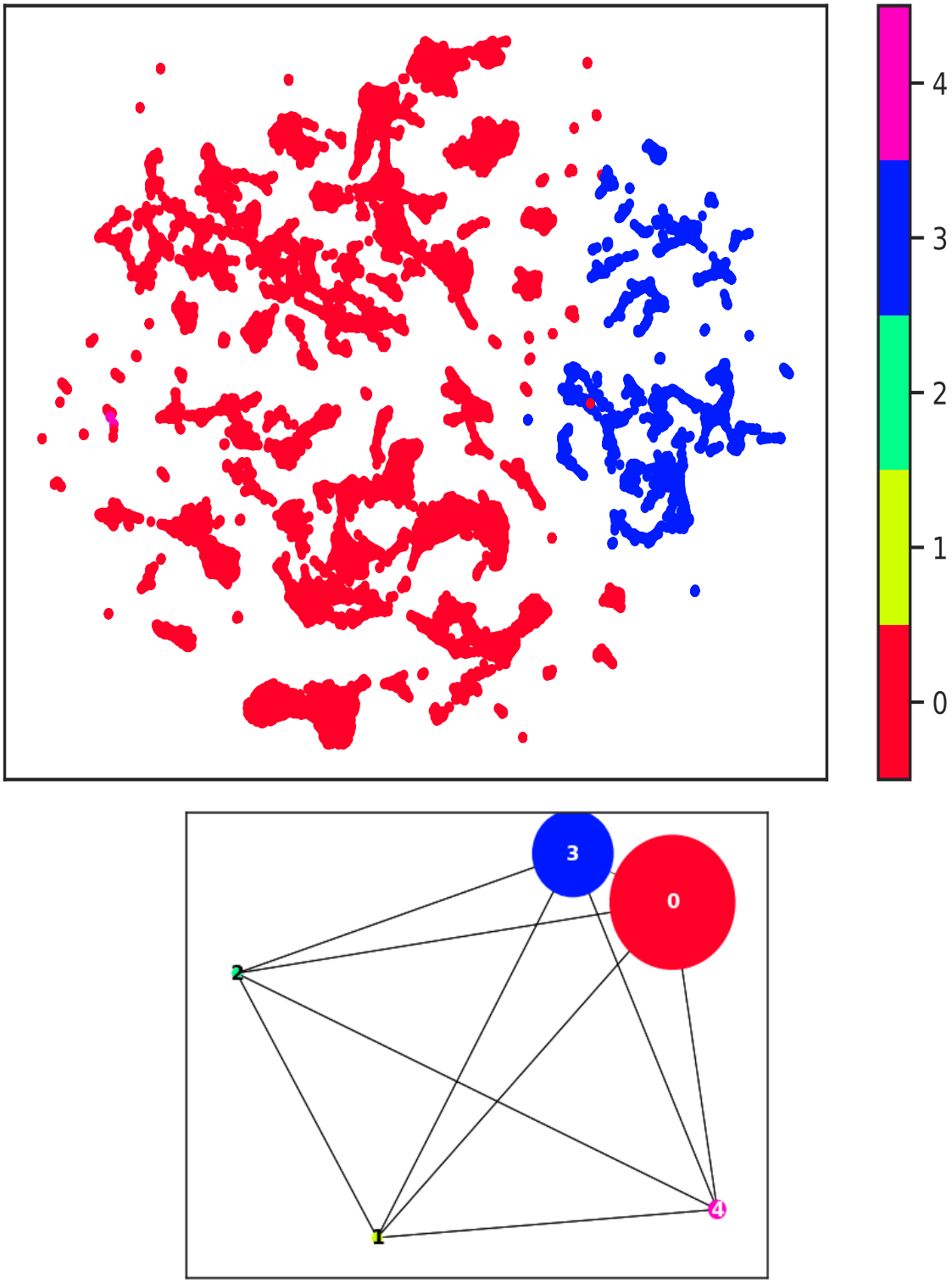

Figure S10: Plot of the DP clustering assignation showing distribution of clusters on a decision graph for V127/VAL129 peptide (upper panel), and a 2D multidimensional scaling projection showing similarity relationships among clusters.