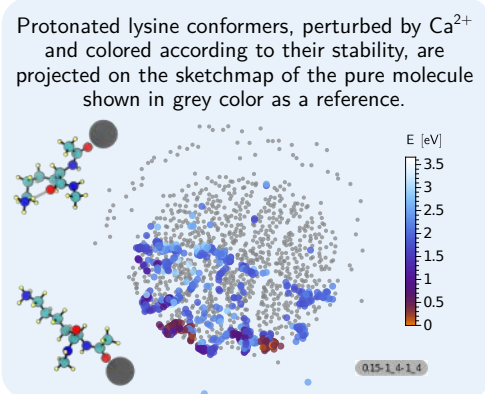
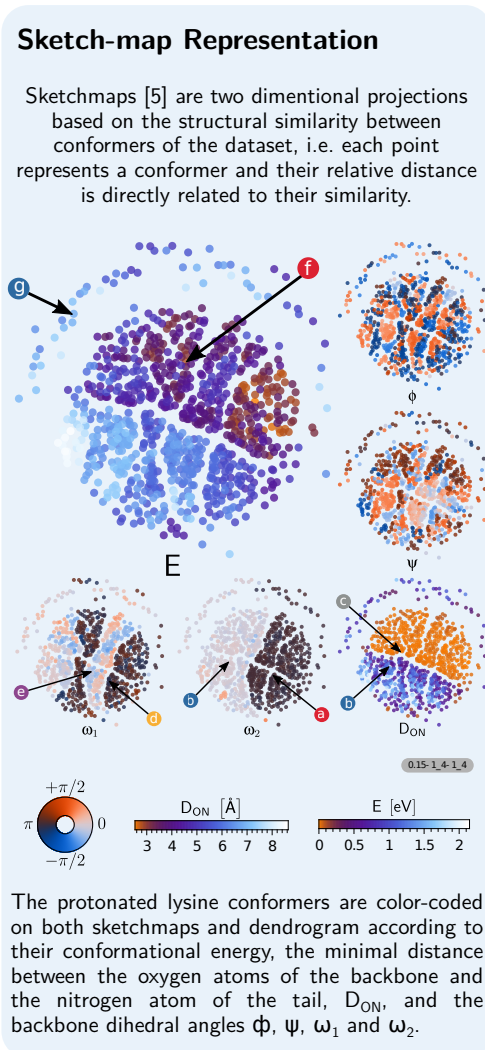
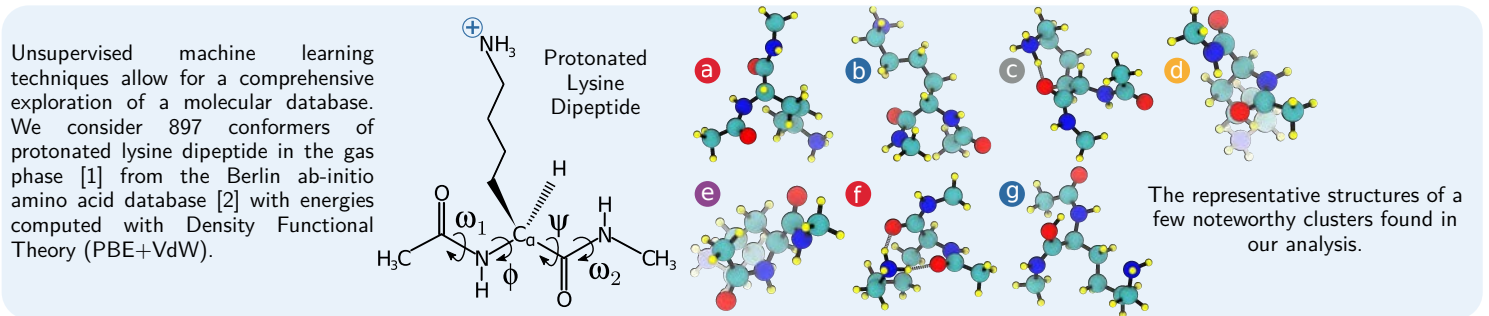


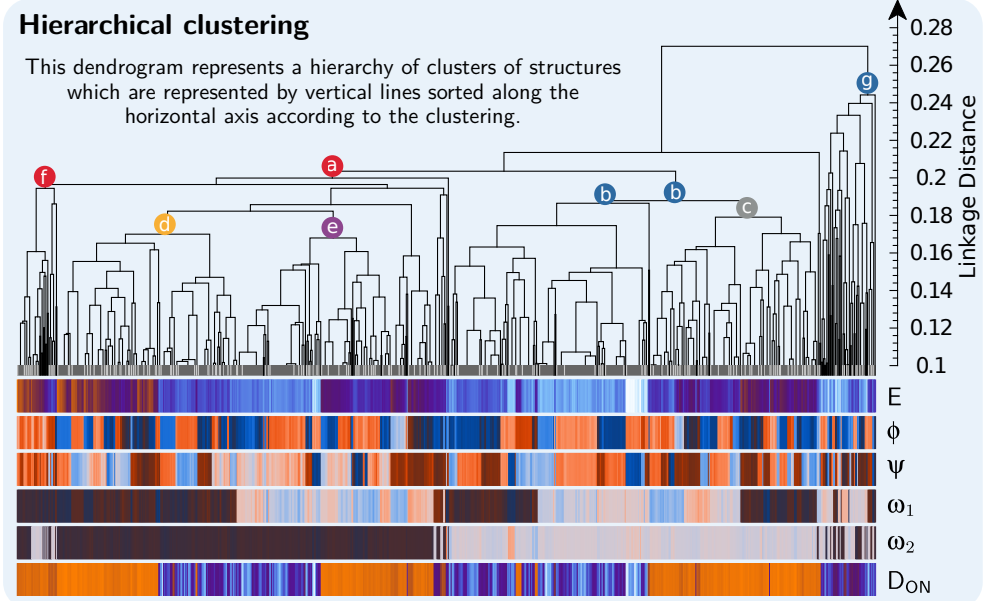
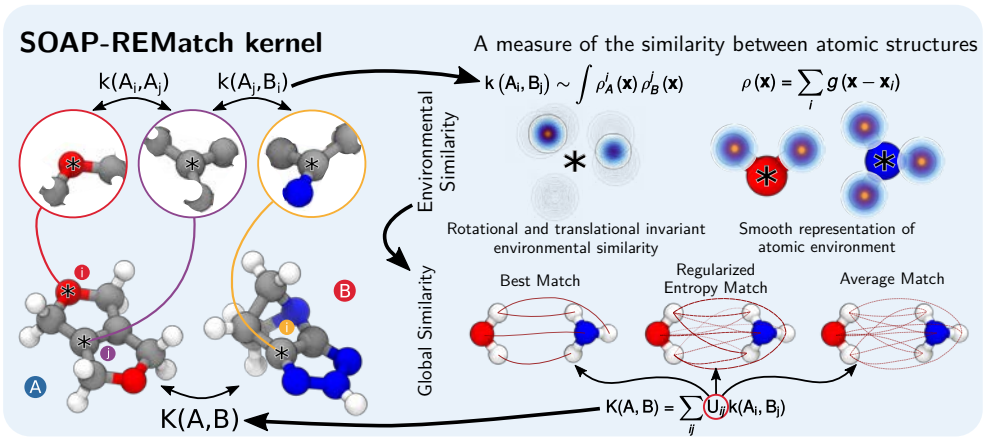
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Physical Insights

Protonated lysine conformers across this dataset are forming structurally-related groups. Investigating the representative structures of these clusters allow for a quick identification of the structural motifs explaining the layout of the conformational landscape:

- The dihedral angles ω_1 and ω_2 forming the four combinations of cis and trans states (see representative structures a-d).
- The distance D_{ON} is directly related to the formation of a H-bond between the tail and the backbone of the amino acid (see representative structures b and c).
- The energetics of the conformers is mainly driven by the extended or bent state of the tail.

The perturbed system is projected on a subset of the original conformational space showing that the Ca^{2+} ion preferably binds to the oxygen atoms of the backbone resulting in extended conformers. An analysis only focused on the Ramachandran dihedrals, ϕ and ψ , would have missed one of the main features of the structural landscape that is critical to characterize the relation between structure and energetics.