

Supporting Information:
Deciphering Amino Acid Adsorption on PVC Surface:
Insights from Molecular Dynamics and PMF
Calculations

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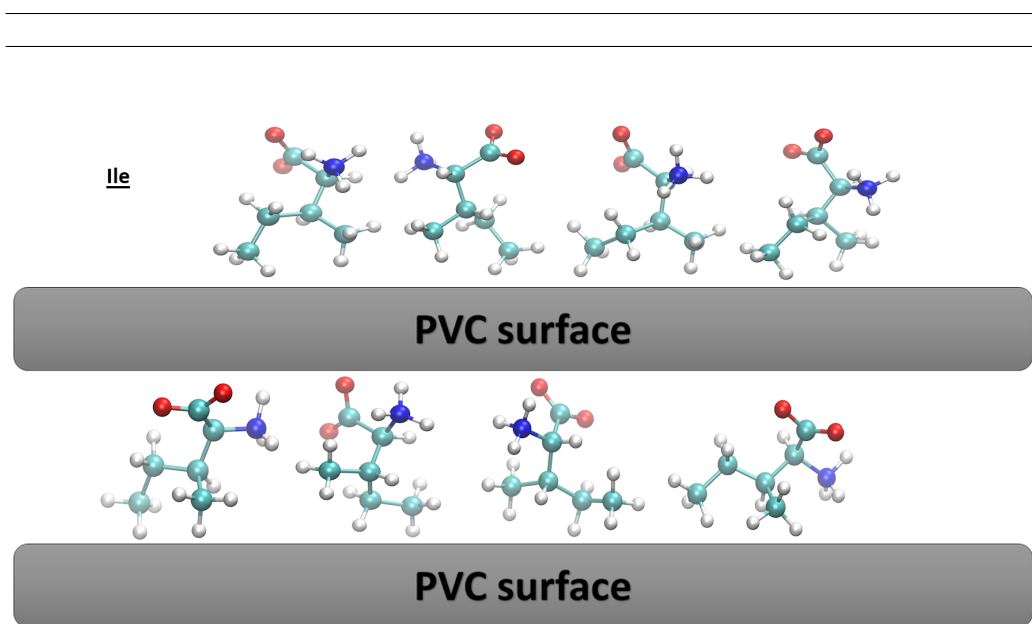


Figure S1: Configuration of the adsorbed Ile residues onto the PVC surface

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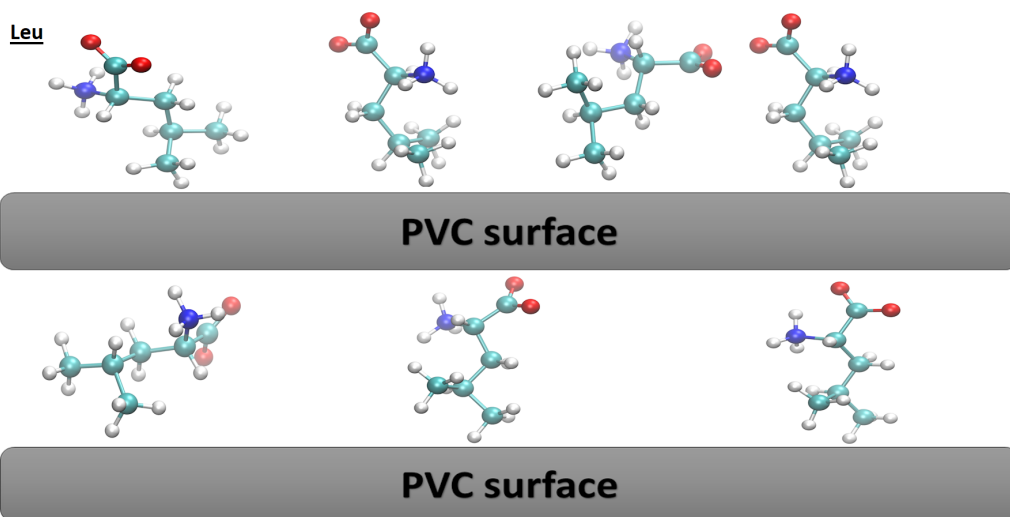


Figure S2: Configuration of the adsorbed Leu residues onto the PVC surface

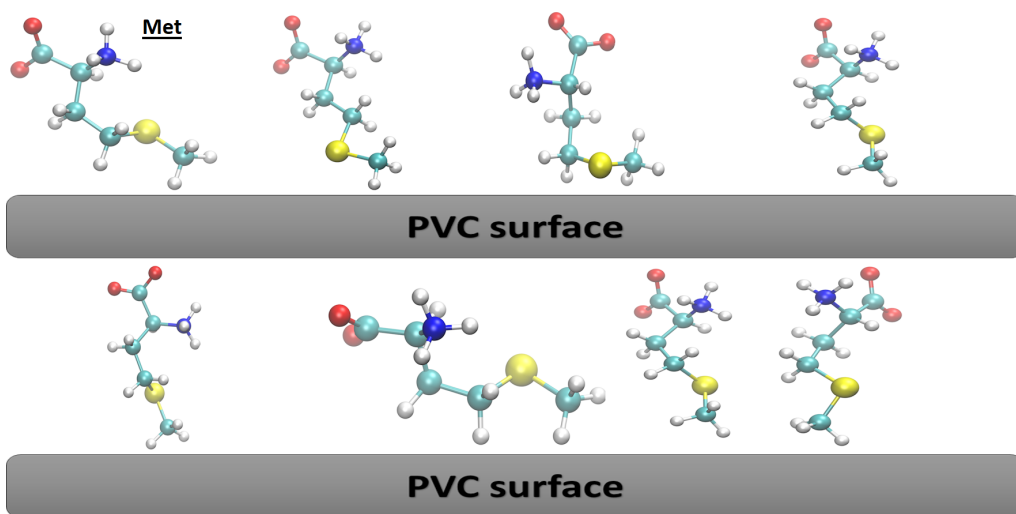


Figure S3: Configuration of the adsorbed Met residues onto the PVC surface

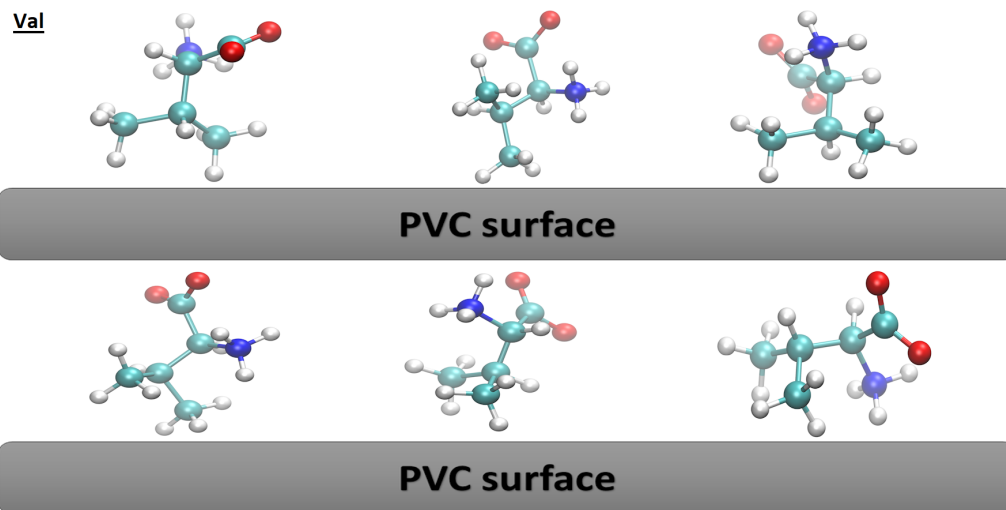


Figure S4: Configuration of the adsorbed Val residues onto the PVC surface

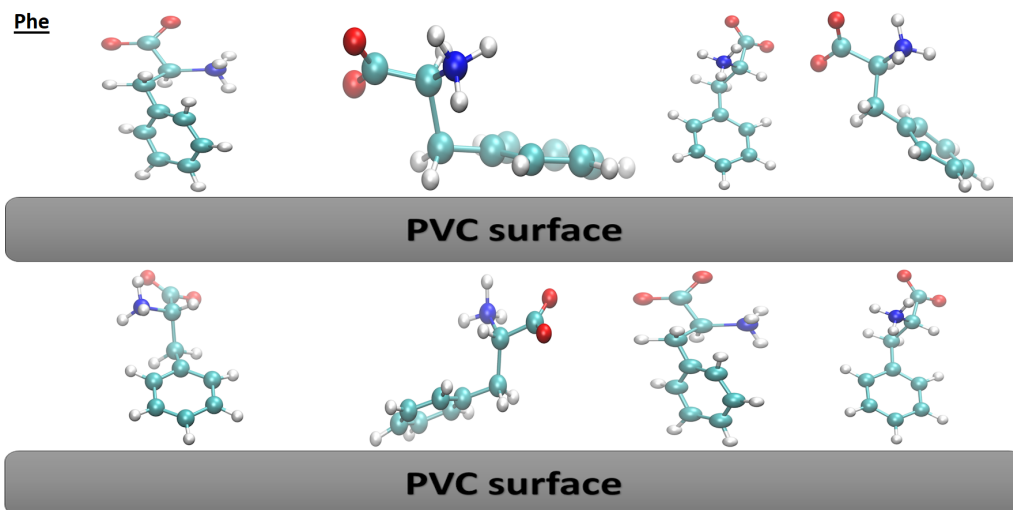


Figure S5: Configuration of the adsorbed Phe residues onto the PVC surface

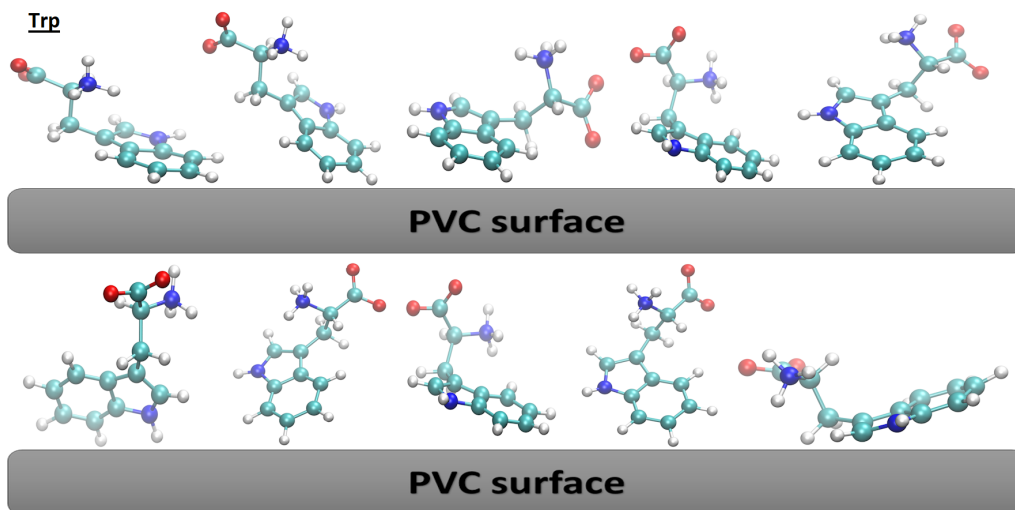


Figure S6: Configuration of the adsorbed Trp residues onto the PVC surface

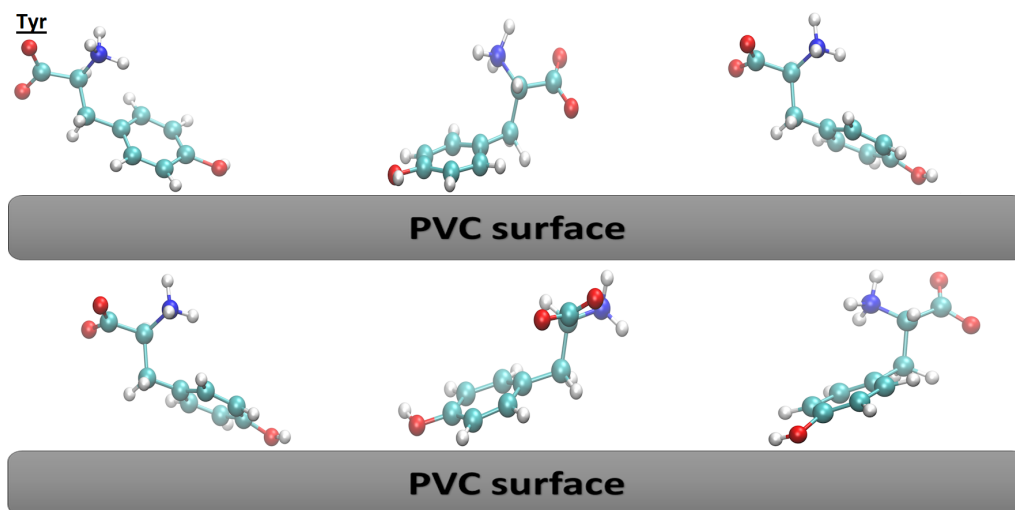


Figure S7: Configuration of the adsorbed Tyr residues onto the PVC surface

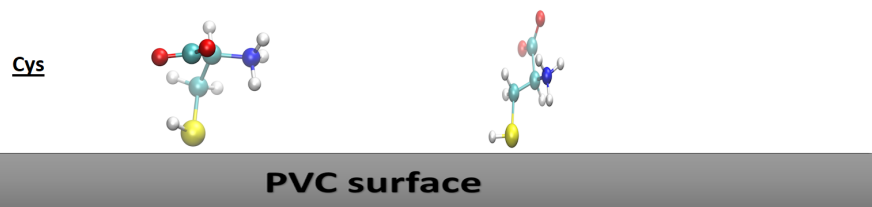


Figure S8: Configuration of the adsorbed Cys residues onto the PVC surface

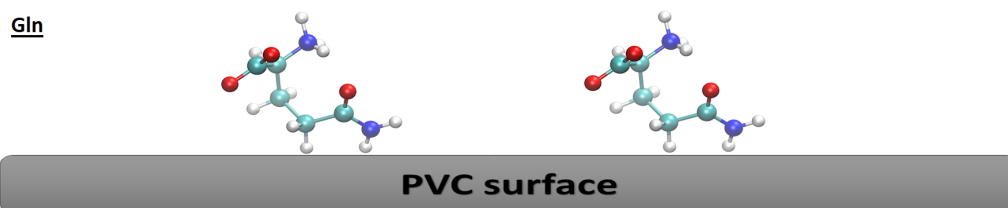


Figure S9: Configuration of the adsorbed Gln residues onto the PVC surface



Figure S10: Configuration of the adsorbed Pro residues onto the PVC surface

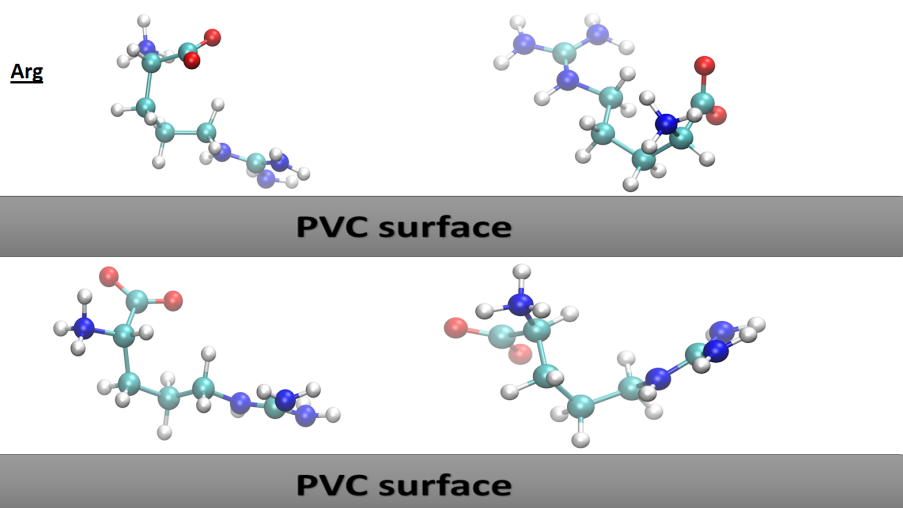


Figure S11: Configuration of the adsorbed Arg residues onto the PVC surface

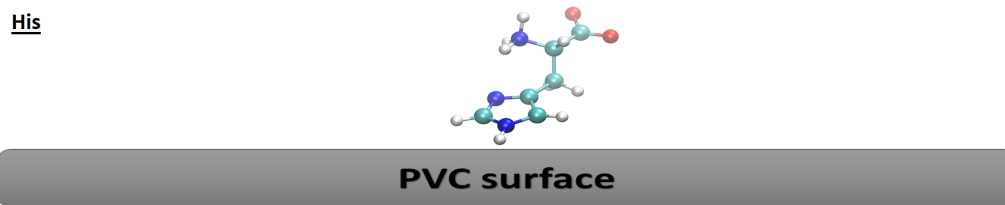


Figure S12: Configuration of the adsorbed His residues onto the PVC surface

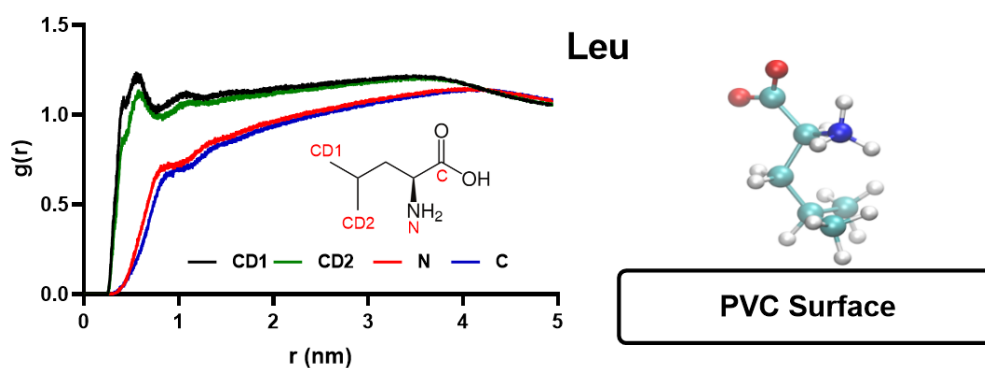


Figure S13: Radial distribution functions ($g(r)$) of the atoms of Leu (left) and the selected orientation of adsorption on PVC surface taken from the last frame of MD simulation (right).

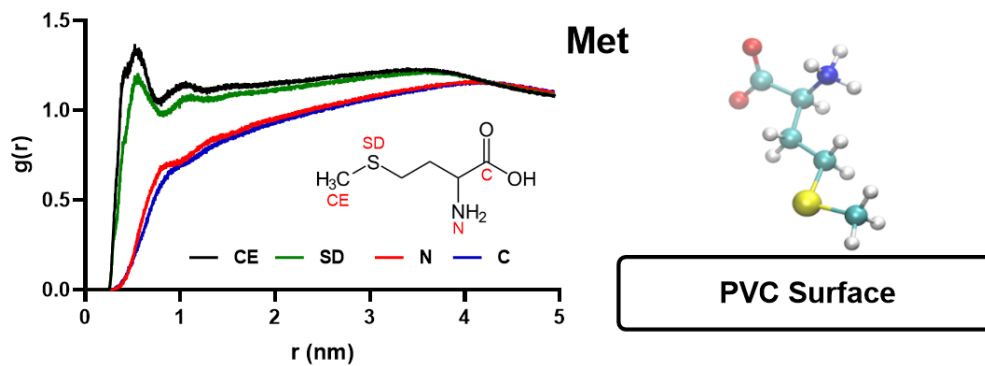


Figure S14: Radial distribution functions ($g(r)$) of the atoms of Met (left) and the selected orientation of adsorption on PVC surface taken from the last frame of MD simulation (right).

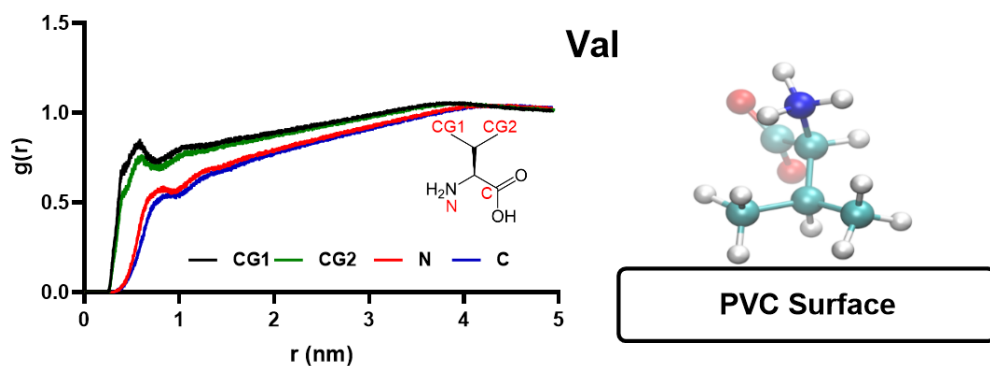


Figure S15: Radial distribution functions ($g(r)$) of the atoms of Val (left) and the selected orientation of adsorption on PVC surface taken from the last frame of MD simulation (right).

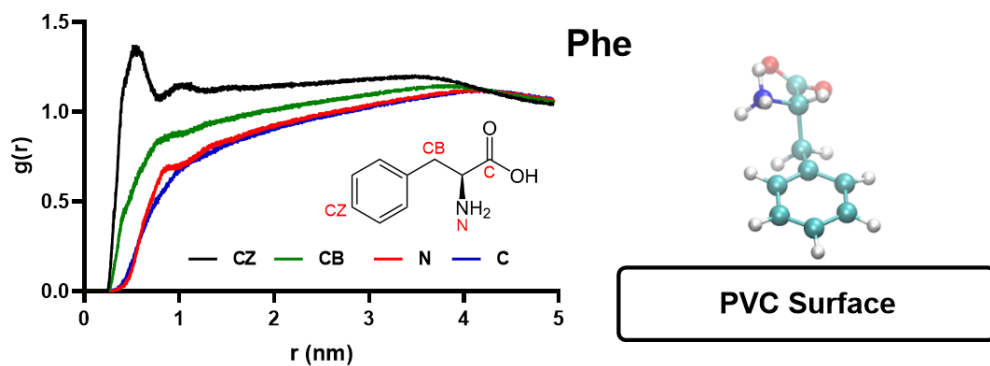


Figure S16: Radial distribution functions ($g(r)$) of the atoms of Phe (left) and the selected orientation of adsorption on PVC surface taken from the last frame of MD simulation (right).

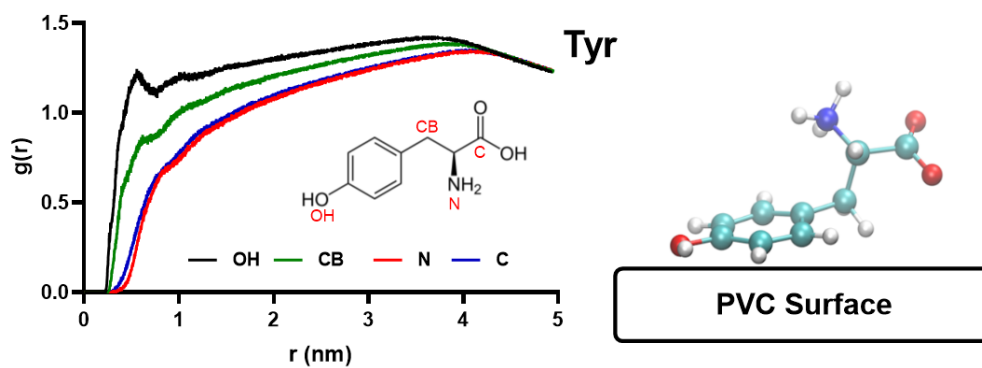


Figure S17: Radial distribution functions ($g(r)$) of the atoms of Tyr (left) and the selected orientation of adsorption on PVC surface taken from the last frame of MD simulation (right).

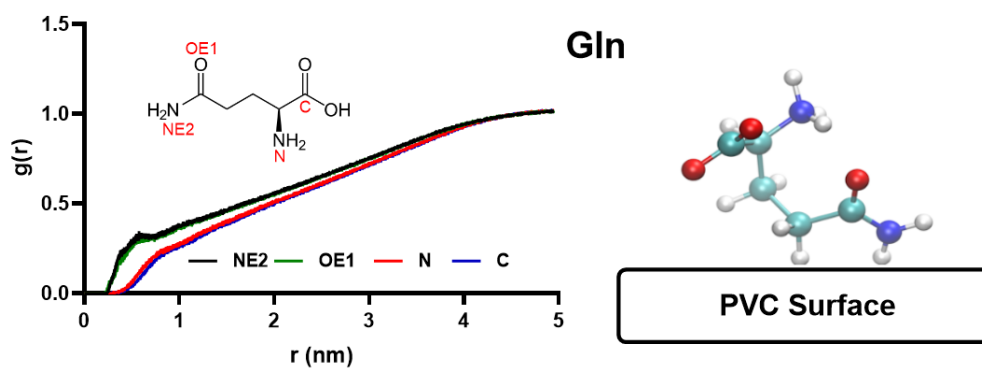


Figure S18: Radial distribution functions ($g(r)$) of the atoms of Gln (left) and the selected orientation of adsorption on PVC surface taken from the last frame of MD simulation (right).

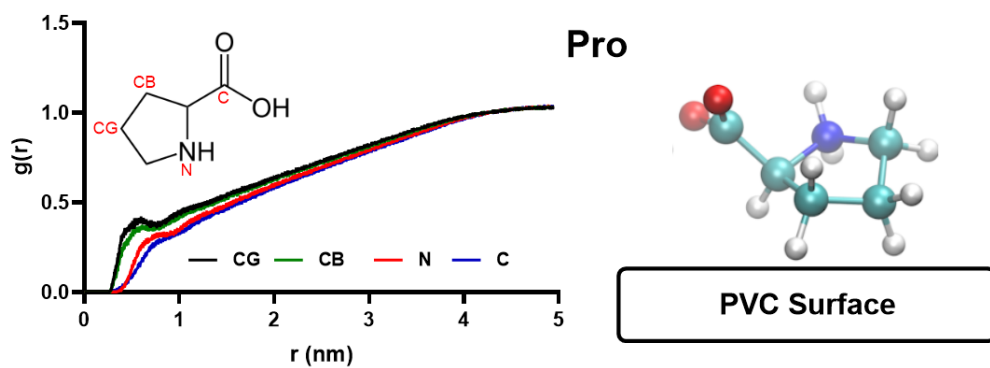


Figure S19: Radial distribution functions ($g(r)$) of the atoms of Pro (left) and the selected orientation of adsorption on PVC surface taken from the last frame of MD simulation (right).

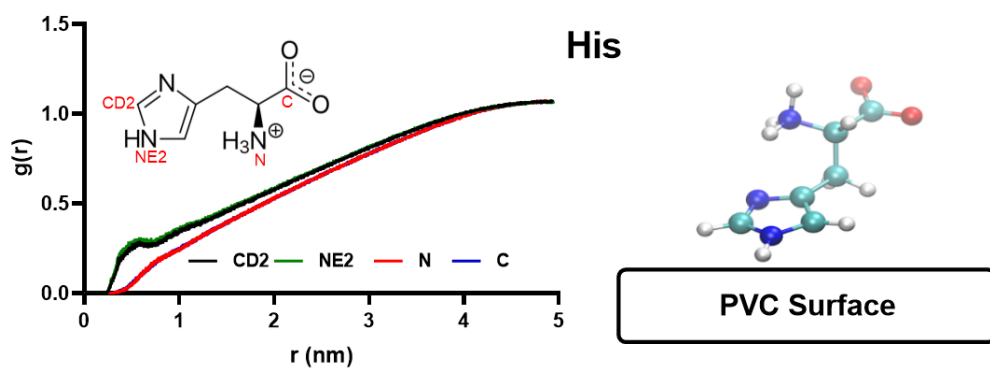


Figure S20: Radial distribution functions ($g(r)$) of the atoms of His (left) and the selected orientation of adsorption on PVC surface taken from the last frame of MD simulation (right).