Machine Learning Models for Predicting Interaction Affinity Energy between Human Serum Proteins and Hemodialysis Membrane Materials

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Table S1. Classification of ligand groups, scaffolds, modification types, and plasma/platelet proteins in the docking dataset.

Ligand Group	Ligand scaffold	Modification type	Proteins
Pure polymers	PES / PAES / PSF / PPSU / PVDF / PAN / PEMA / PMEA / Cellulose / Cellulose monoacetate / Cellulose diacetate / CTA	None	Alb/ FB/ TR/ Hem/ HSP/ P2Y12*
ZWs	Different zwitterionic materials (e.g., SBMA, CBMA, MPC, MMP, and other zwitterionic modifiers)	None	
Zwitterionic modified	PES / PSF / PPSU / PVDF / Cellulose / Cellulose monoacetate / Cellulose diacetate / CTA / PVP-containing systems	Single zwitterionic material per scaffold	
Linker	Individual linker molecules (e.g., guanidine, guanidinoacetic acid, vinyl chloride, urea, and different uremic-metabolite-based linkers)	None	
Cation	Standalone cationic ligands (e.g., diallyl ammonium chloride)	None	
Cation-modified	PES / PSF / PPSU / PVDF / Cellulose / Cellulose monoacetate / Cellulose diacetate / CTA / PVP-containing systems	Single cationic ligand per scaffold	
Anion	Standalone anionic ligands (e.g., vinybenzoic acid)	None	
Anion-modified	PES / PSF / PPSU / PVDF / Cellulose / Cellulose monoacetate / Cellulose diacetate / CTA / PVP-containing systems	Single anionic ligand per scaffold	
Mixed systems	PES / PSF / PPSU / PVDF / Cellulose / Cellulose monoacetate / Cellulose diacetate / CTA / PVP-containing systems	Combinations of cationic, anionic, and/or zwitterionic modifiers, with or without linker molecules	

*All ligand categories were docked against Alb, FB, TR, Hem, HSP, and P2Y12.

Table S2. Qualitative summary of chemical descriptor space represented in the ligand dataset

Category	**Description**
Molecular weight coverage	Small to large molecules
Atom count coverage	Low to high complexity
Hydrophilicity spread	Super-hydrophobic to super-hydrophilic
Charge diversity	− / 0 / + / zwitterionic