Molecular Modeling to Provide Insight into the Substrate Binding and Catalytic Mechanism of Human Biliverdin-IXα Reductase

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Supporting Information

Table S1. Different components of residue-based binding free energies for the five ternary complexes of hBVR-A/NADPH/substrates.

Residue	ΔG_{vdW}	ΔG_{elec}	$\Delta G_{solv\text{-}pol}$	$\Delta G_{solv\text{-}nonpol}$	ΔG_{bind}
Substrate **I**					
Tyr98	−1.48	−4.19	3.75	−0.10	−2.02
Arg172	−0.04	−72.09	63.45	−0.02	−8.07
Arg225	−2.47	−96.02	82.00	−0.53	−17.03
Arg227	−0.15	−56.84	52.67	−0.01	−4.33
Substrate **II**					
Tyr98	−1.68	0.56	−0.34	−0.11	−1.57
Arg172	0.46	−83.71	68.33	−0.05	−14.97
Arg225	−3.13	−80.96	73.86	−0.52	−10.75
Arg227	0.15	−59.44	53.78	−0.05	−5.56
Substrate **III**					
Tyr98	−1.39	0.77	0.44	−0.09	−0.27
Arg172	−0.89	−43.80	37.51	−0.14	−7.31
Arg225	−3.54	−40.58	38.76	−0.56	−5.92
Arg227	−0.30	−26.98	25.82	−0.05	−1.51
Substrate **IV**					
Tyr98	−0.90	0.47	0.13	−0.08	−0.38
Arg172	0.03	−73.41	62.84	−0.07	−10.60
Arg225	−4.00	−89.62	79.48	−0.67	−14.81
Arg227	−0.19	−48.11	45.94	−0.06	−2.42
Substrate **V**					
Tyr98	−1.30	−4.08	3.52	−0.16	−2.02
Arg172	−0.52	−73.82	68.10	−0.04	−6.27
Arg225	−2.39	−89.39	81.44	−0.57	−10.90
Arg227	−0.04	−65.62	62.63	−0.10	−3.12

Table S2. Important hydrogen bonding interactions between the conserved water molecules and Substrate **I** and NADPH during the production phase of MD simulations.

Donor	Acceptor	Distance (Å) (SD)	Angle (°) (SD)	Occupancy (%)
Substrate **I** N_2-H_{11}	Water O	3.00 (0.16)	27.46 (14.28)	27.78
Water H_1	NADPH C=O	2.72 (0.13)	19.42 (12.45)	16.67
Water H_2	NADPH C=O	2.70 (0.13)	16.50 (9.15)	13.61