Fig S1: Simulations protocol for the role of protonation state and electrostatic charges on the conformation and dynamics of albumin structure.
Fig S2: 3D structure of BSA (4F5S.pdb)

Fig S3: 3D structure of Simulated BSA at 10mM and pH 2
Fig S4: 3D structure of Simulated BSA at 10mM and pH 3.5

Fig S5: 3D structure of Simulated BSA at 10mM and pH 4.3
Fig S6: 3D structure of Simulated BSA at 10mM and pH 7.4

Fig S7: 3D structure of Simulated BSA at 10mM and pH 9.0
Fig S8: 3D structure of Simulated BSA at 20mM and pH 2.0

Fig S9: 3D structure of Simulated BSA at 20mM and pH 3.5
Fig S10: 3D structure of Simulated BSA at 20mM and pH 4.3

Fig S11: 3D structure of Simulated BSA at 20mM and pH 7.4
Fig S12: 3D structure of Simulated BSA at 20mM and pH 9.0

Fig S13: 3D structure of Simulated BSA at 30mM and pH 2.0
Fig S14: 3D structure of Simulated BSA at 30mM and pH 3.5

Fig S15: 3D structure of Simulated BSA at 30mM and pH 4.3
Fig S16: 3D structure of Simulated BSA at 30mM and pH 7.4

Fig S17: 3D structure of Simulated BSA at 30mM and pH 9.0
Fig S18: 3D structure of Simulated BSA at 40 mM and pH 2.0

Fig S19: 3D structure of Simulated BSA at 40 mM and pH 3.5
Fig S20: 3D structure of Simulated BSA at 40 mM and pH 4.3

Fig S21: 3D structure of Simulated BSA at 40 mM and pH 7.4
Fig S22: 3D structure of Simulated BSA at 40 mM and pH 9.0

Fig S23: 3D structure of Simulated BSA at 50 mM and pH 2.0
Fig S24: 3D structure of Simulated BSA at 50 mM and pH 3.5

Fig S25: 3D structure of Simulated BSA at 50 mM and pH 4.3
Fig S26: 3D structure of Simulated BSA at 50 mM and pH 7.4

Fig S27: 3D structure of Simulated BSA at 50 mM and pH 9.0
Fig S28: Ramachandran Plot of Simulated BSA at 10 mM and pH 2.0

Fig S29: Ramachandran Plot of Simulated BSA at 10 mM and pH 3.5

Fig S30: Ramachandran Plot of Simulated BSA at 10 mM and pH 4.3

Fig S31: Ramachandran Plot of Simulated BSA at 10 mM and pH 7.4
Fig S32: Ramachandran Plot of Simulated BSA at 10 mM and pH 9.0

Fig S33: Ramachandran Plot of Simulated BSA at 20 mM and pH 2.0

Fig S34: Ramachandran Plot of Simulated BSA at 20 mM and pH 3.5

Fig S35: Ramachandran Plot of Simulated BSA at 20 mM and pH 4.3
Fig S36: Ramachandran Plot of Simulated BSA at 20 mM and pH 7.4

Fig S37: Ramachandran Plot of Simulated BSA at 20 mM and pH 9.0

Fig S38: Ramachandran Plot of Simulated BSA at 30 mM and pH 2.0

Fig S39: Ramachandran Plot of Simulated BSA at 30 mM and pH 3.5
Fig S40: Ramachandran Plot of Simulated BSA at 30 mM and pH 4.3

Fig S41: Ramachandran Plot of Simulated BSA at 30 mM and pH 7.4

Fig S42: Ramachandran Plot of Simulated BSA at 30 mM and pH 9.0

Fig S43: Ramachandran Plot of Simulated BSA at 40 mM and pH 2.0
Fig S44: Ramachandran Plot of Simulated BSA at 40 mM and pH 3.5

Fig S45: Ramachandran Plot of Simulated BSA at 40 mM and pH 4.3

Fig S46: Ramachandran Plot of Simulated BSA at 40 mM and pH 7.4

Fig S47: Ramachandran Plot of Simulated BSA at 40 mM and pH 9.0
Fig S48: Ramachandran Plot of Simulated BSA at 50 mM and pH 2.0

Fig S49: Ramachandran Plot of Simulated BSA at 50 mM and pH 3.5

Fig S50: Ramachandran Plot of Simulated BSA at 50 mM and pH 4.3

Fig S51: Ramachandran Plot of Simulated BSA at 50 mM and pH 7.4
Fig S52: Ramachandran Plot of Simulated BSA at 50 mM and pH 9.0