Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Theoretical Design of Imprinted Albumin against Foodborne Toxins

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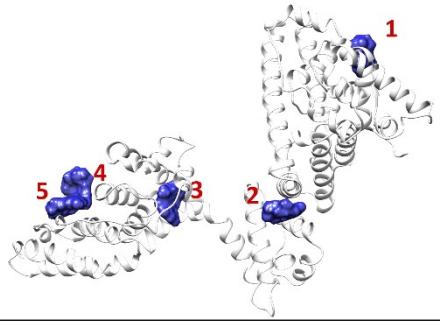
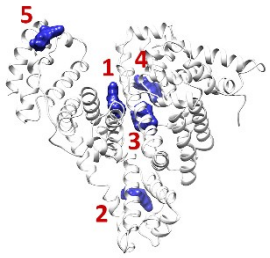
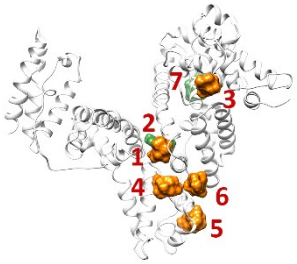
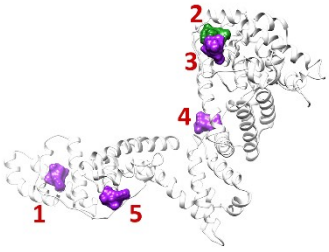
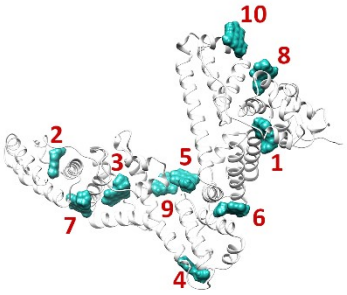
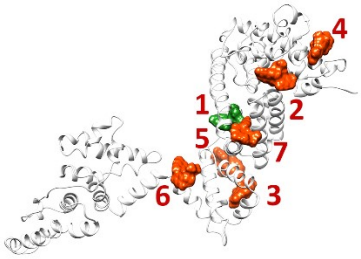
Table S1. Secondary structure (α-helix content, %) of the BSA at different pH values

pH	Modelling	Method of Greenfield and Fasman
3.0	55.1	54.5
7.4	67.2	68.9

Table S2. Solvent accessible surface area (SASA) of the Trp residues of BSA at various pH values

Residue	Trp134		Trp213	
	pH 7.4	pH 3.0	pH 7.4	pH 3.0
SASA (Non-polar)	11.05	41.05	19.85	71.18
SASA (Polar)	0	0	16.92	14.33
SASA	11.05	41.05	36.75	85.51

Table S3. Free binding energy of BSA-template complexes at pH 3.0

Template molecule	$\Delta G_{MM\text{-}GBSA}$, kcal/mol	Complex BSA—template
ZEA	**1:** -33.8 **2:** -40.9 **3:** -47.8 **4:** -35.1 **5:** -25.7	
ZEA (pH 7.4)	**1:** -40.3 **2:** -37.9 **3:** -28.6 **4:** -23.9 **5:** -23.5	
DON	**1:** -49.8 **2:** -46.5 **3:** -39.0 **4:** -36.7 **5:** -33.8 **6:** -31.6 **7:** -23.3	
DOM-1	**1:** -50.5 **2:** -39.3 **3:** -36.0 **4:** -29.3 **5:** -21.7	
AFB-1	**1:** -65.9 **2:** -56.3 **3:** -51.9 **4:** -43.2 **5:** -41.5 **6:** -41.4 **7:** -38.7 **8:** -34.7 **9:** -34.7 **10:** -26.5	
KWA	**1:** -59.8 **2:** -53.6 **3:** -40.8 **4:** -40.5 **5:** -37.6 **6:** -30.5 **7:** -23.6	

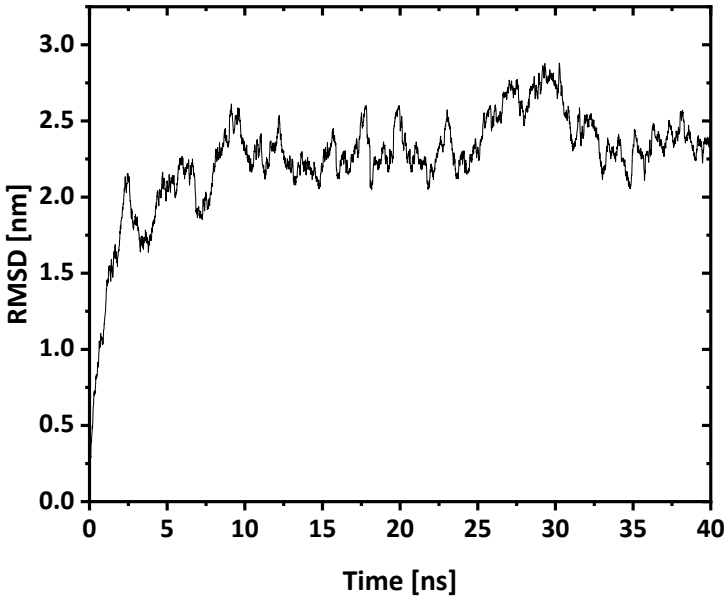
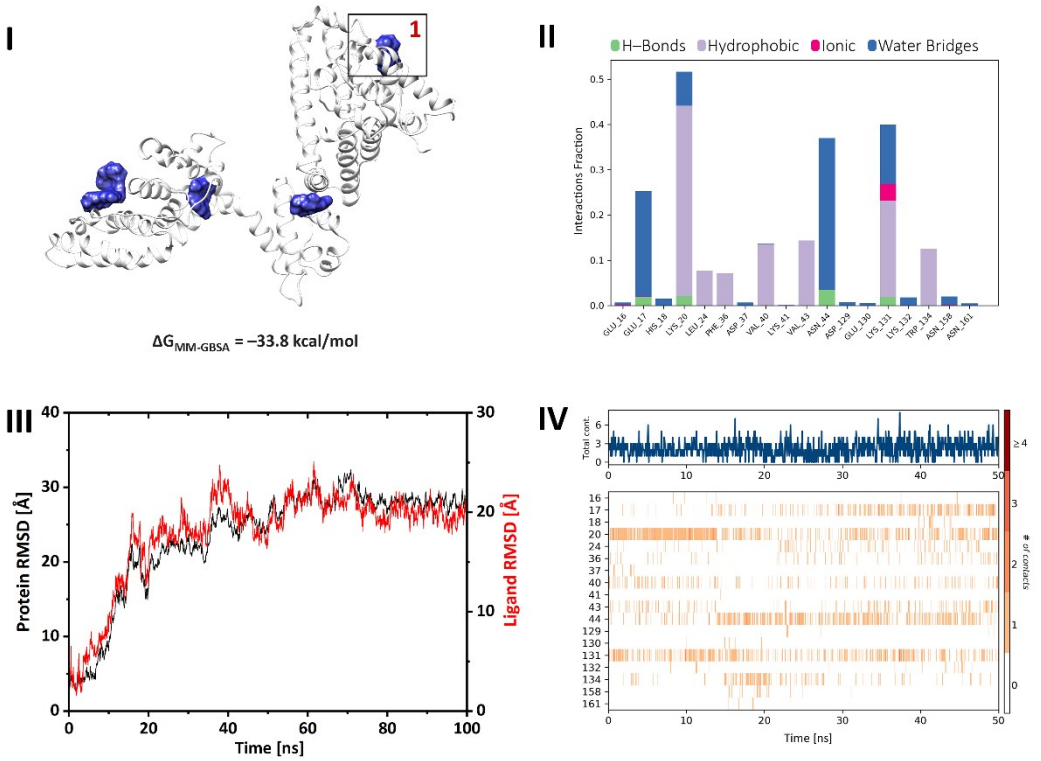
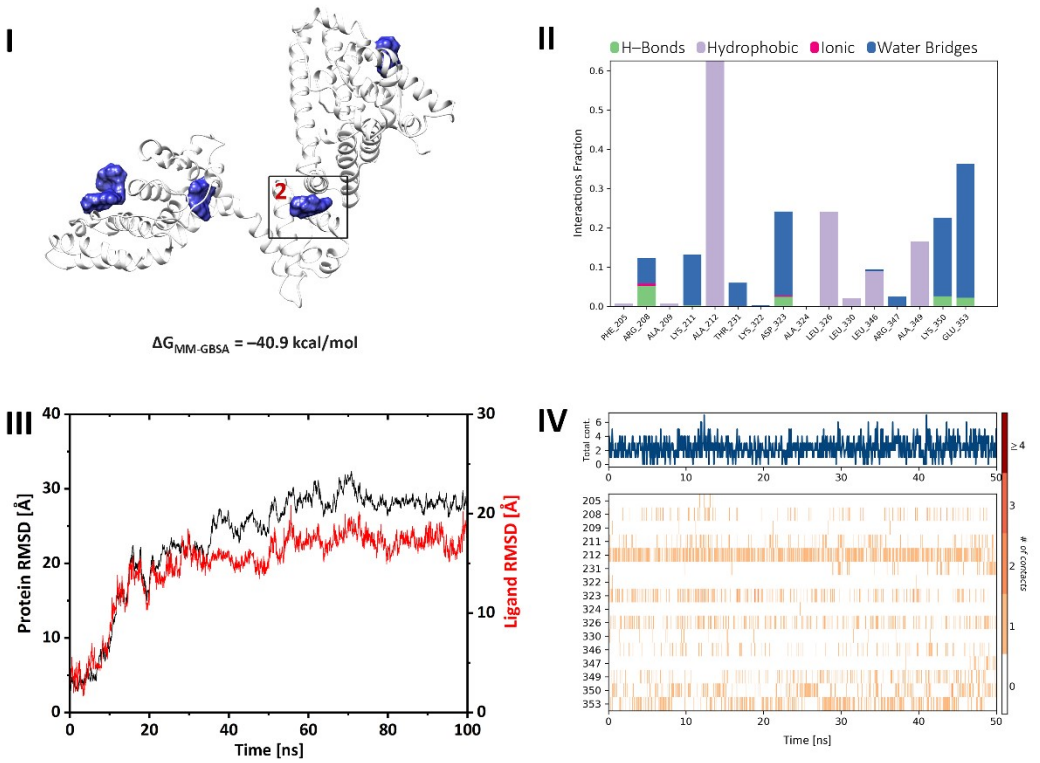


Fig.S1. RMSD of BSA during molecular dynamics simulation.

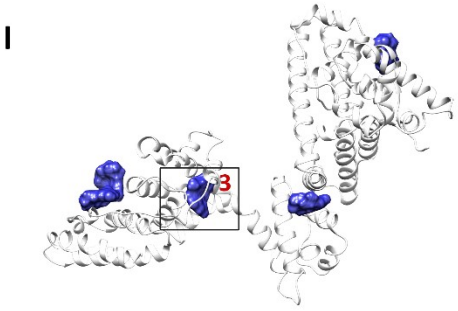
A


I
1
ΔG MM-GBSA = −33.8 kcal/mol
II
H–Bonds
Hydrophobic
Ionic
Water Bridges
Interactions Fraction
GLU_16
GLU_17
HIS_18
LYS_20
LEU_24
PHE_36
ASP_37
VAL_40
LYS_41
VAL_43
ASN_44
ASP_129
GLU_130
LYS_131
LYS_132
TRP_134
ASN_158
ASN_161
III
Protein RMSD [Å]
Ligand RMSD [Å]
Time [ns]
IV
Total cont.
# of contacts
Time [ns]

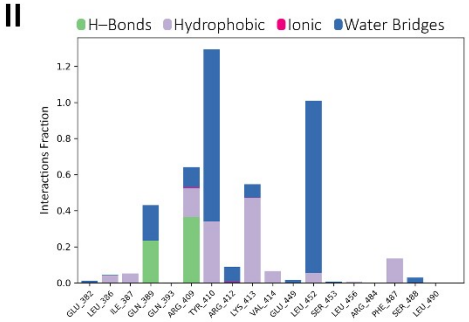
B

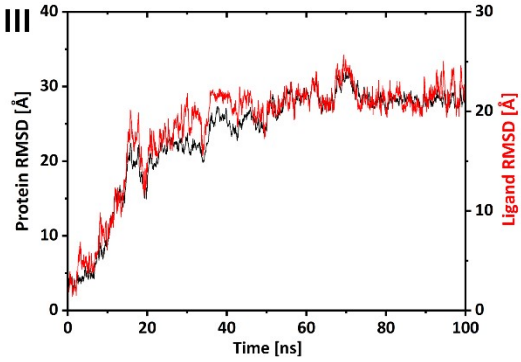

I
2
ΔG MM-GBSA = −40.9 kcal/mol
II
H–Bonds
Hydrophobic
Ionic
Water Bridges
Interactions Fraction
PHE_205
ARG_208
ALA_209
LYS_211
ALA_212
THR_231
LYS_322
ASP_323
ALA_324
LEU_326
LEU_330
LEU_346
ARG_347
ALA_349
LYS_350
GLU_353
III
Protein RMSD [Å]
Ligand RMSD [Å]
Time [ns]
IV
Total cont.
# of contacts
Time [ns]

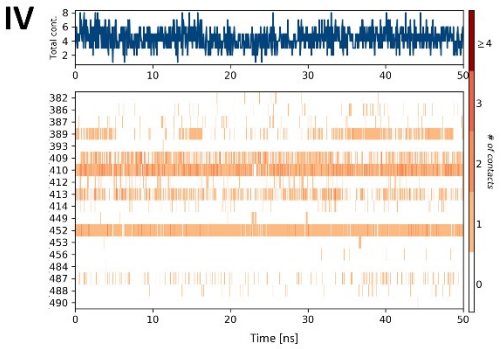
C



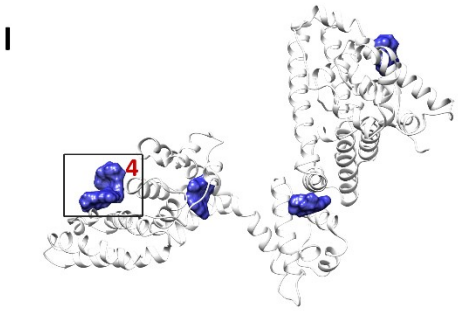
$\Delta G_{MM\text{-}GBSA}$ = −47.8 kcal/mol



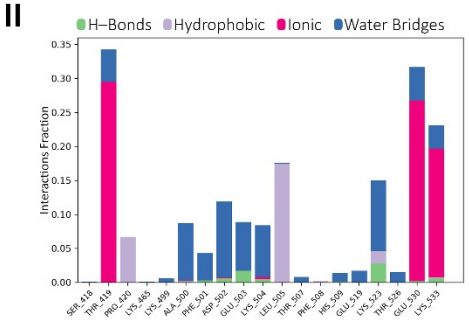


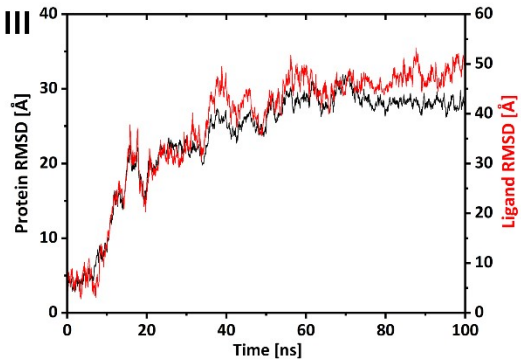


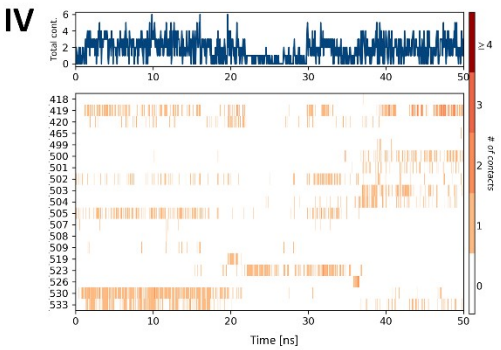
D



$\Delta G_{MM\text{-}GBSA}$ = −35.1 kcal/mol







E

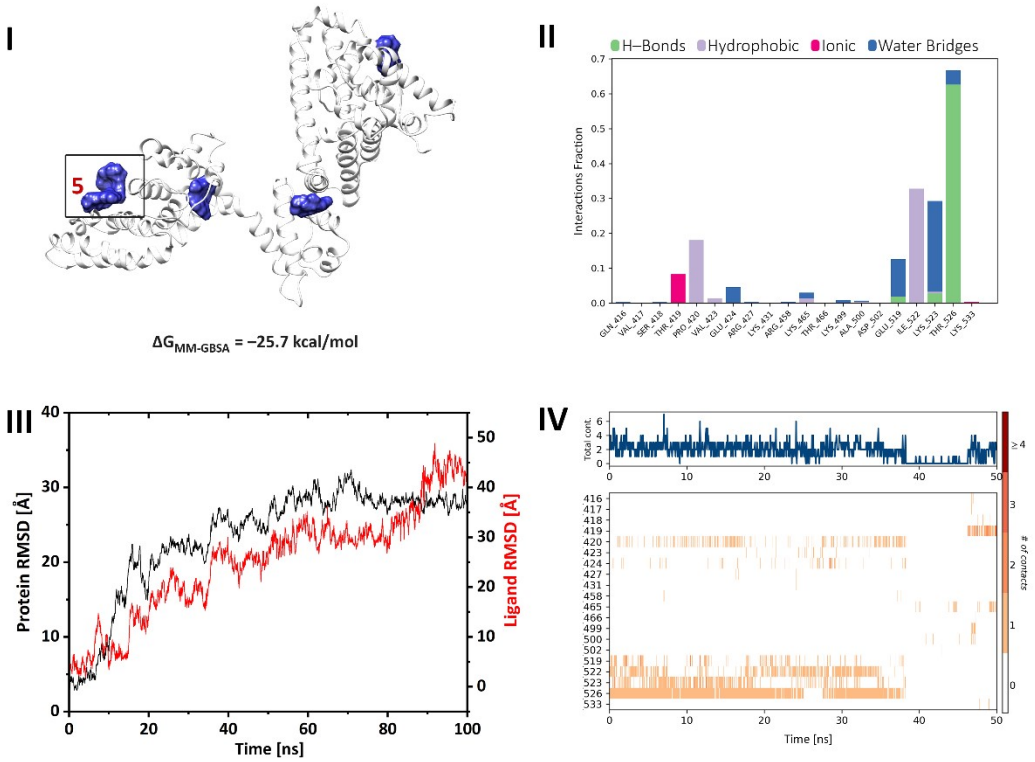


Fig.S2. Results of molecular modelling of BSA-ZEA complex at pH 3.0: (I) location of ZEA in the supposed binding site; (II) protein–ligand interactions percentage; (III) system RMSD; (IV) the intensity of contacts between the ligand and amino acids during simulation time.