Supplementary data

Supplementary Tables

supplementary Table S1. Predicted bonds between interacting atoms of different amino acids of ***α***-glucosidase [PDB ID: 3A4A] and coumarin.

S. No.	Amino acids	Distance (A°)	Nature of interaction
1.	Lys156	5.94	Hydrogen bond
2.	Ile419	5.26	Hydrophobic
3.	His423	3.13	Electrostatic interaction
4.	Glu422	4.24	Electrostatic interaction
5.	Ala418		van der Waals force
6.	Glu429		van der Waals force
7.	Asp233		van der Waals force
8.	Trp238		van der Waals force

supplementary Table S2. Changes in accessible surface area (ΔASA) in Å^2 for the ***α***-glucosidase residues interacting with coumarin.

S. No.	Residues	ASA (Å^2) in ***α***-glucosidase	ASA (Å^2) in ***α***-glucosidase – Coumarin complex	ΔASA (Å^2)
1.	Lys156	46.717	31.053	15.664
2.	Asp233	21.153	10.916	10.237
3.	Ser236	19.714	11.933	7.781
4.	Trp238	53.766	53.559	0.207
5.	Ala418	12.143	5.901	6.242
6.	Ile419	13.278	0.00	13.278
7.	Glu422	57.516	47.612	9.904
8.	His 423	53.945	44.477	9.468
9.	Glu429	54.6	39.222	15.378

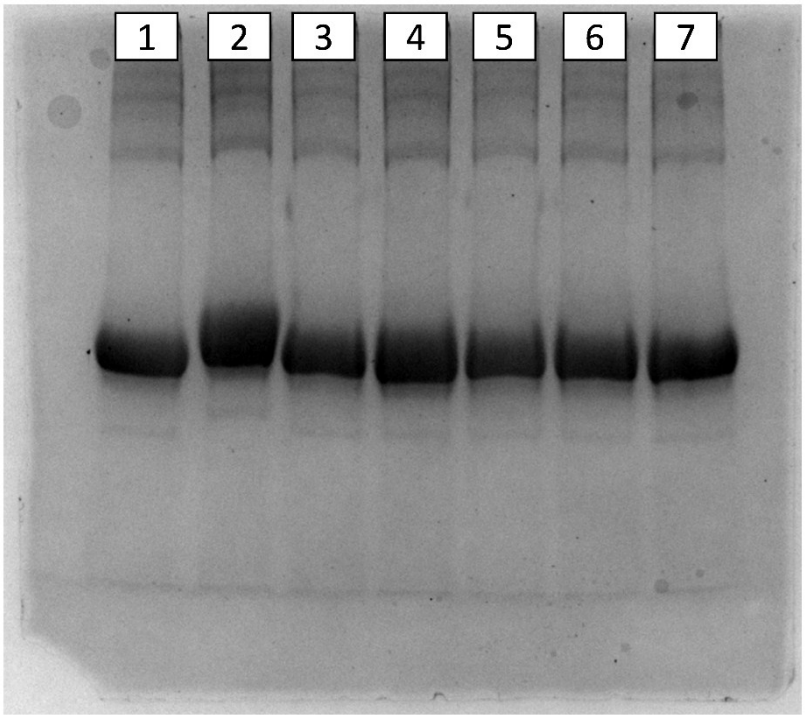
Supplementary table S3. Predicted bonds between interacting atoms of different amino acids of HSA [PDB ID: 1AO6] and coumarin.

S. No.	Domain	Amino acids	Distance (A°)	Nature of interaction
1.	IIA	Arg257	5.28	Hydrophobic
2.	IIA	Ala261	5.23	Hydrophobic
3.	IIA	Leu238	3.85	Hydrophobic
4.	IIA	Leu260	4.84	Hydrophobic
5.	IIA	Ile290	3.92	Hydrophobic
6.	IIA	Ala291	4.69	Hydrophobic
7.	IIA	Ile264		van der Waals force
8.	IIA	Ser 287		van der Waals force
9.	IIA	Arg222		van der Waals force

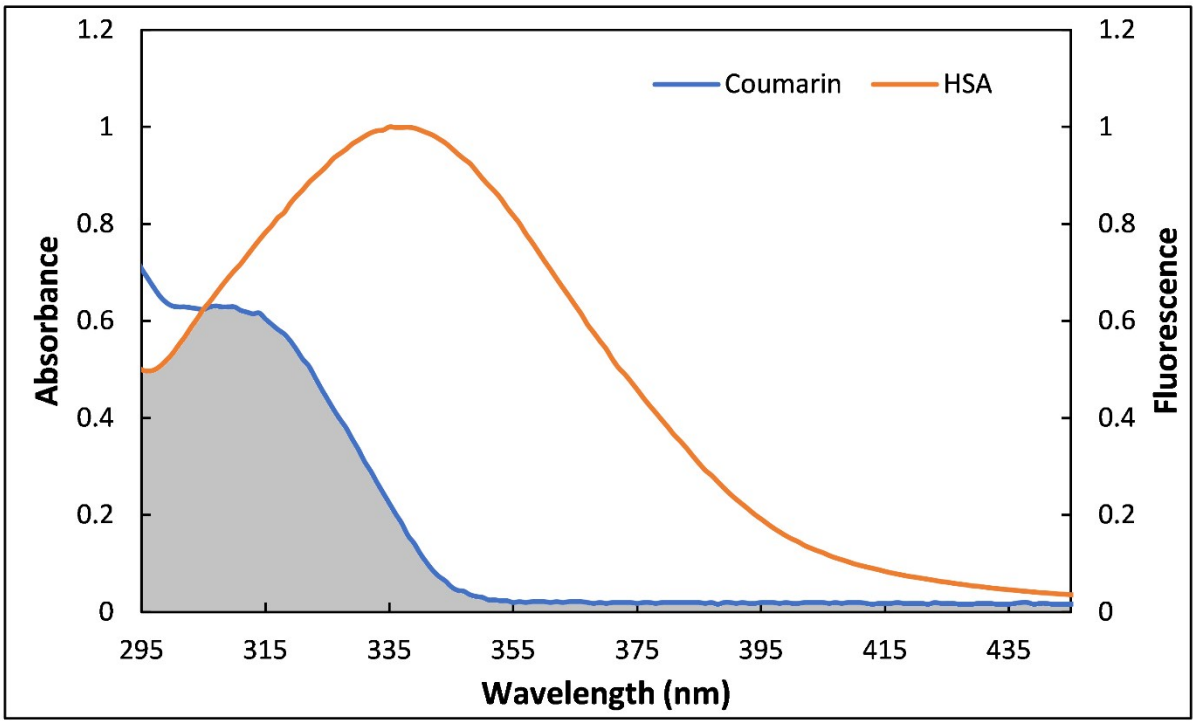
supplementary Table S4. Changes in accessible surface area (ΔASA) in Å^2 for the HSA residues interacting with coumarin.

S. No.	Residues	ASA (Å^2) in HSA	ASA (Å^2) in HSA–Coumarin complex	ΔASA (Å^2)	Domain
1.	Arg222	31.178	20.651	10.527	IIA
2.	Leu238	30.529	0	30.529	IIA
3.	Arg257	15.368	5.231	10.137	IIA
4.	Leu260	15.548	4.426	11.122	IIA
5.	Ala261	3.405	0.113	3.292	IIA
6.	Ile264	9.647	0	9.647	IIA
7.	Ser287	6.395	3.007	3.388	IIA
8.	Ile290	12.978	0.19	12.788	IIA
9.	Ala291	40.991	15.578	25.413	IIA

Supplementary Figures



Supplementary Fig S1. SDS-polyacrylamide gel electrophoresis of HSA on 8% SDS-PAGE for 4 h at 80 V. Protein samples (10 µg in each lane) were loaded on well. Lanes: (1) native HSA; (2) glycated HSA; (3) aminoguanidine; (4) 50 µM; (5) 100 µM; (6) 200 µM; (7) 500 µM coumarin respectively.



Supplementary Fig S2. Spectral overlaps of absorption spectra of coumarin (blue) with fluorescence emission spectra of HSA (orange).