Deciphering the interaction of plumbagin with human serum albumin: A combined biophysical and molecular docking study

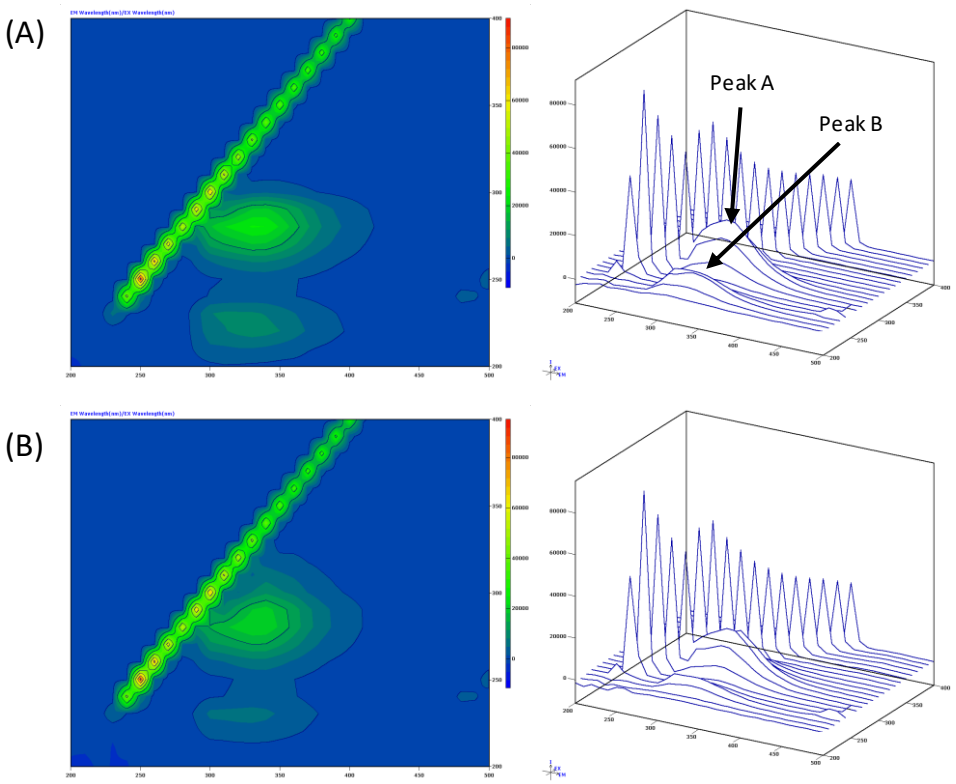
Faizan Abul Qais[1], **Fohad Mabood Husain**[2] **Rais Ahmad Khan**[3*], **Iqbal Ahmad**[1], and **Iftekhar Hassan**[4]

[1]*Department of Agricultural Microbiology, Faculty of Agricultural Sciences, Aligarh Muslim University, Aligarh, India.*
[2]*Department of Food Science and Nutrition, College of Food and Agriculture Science, King Saud University, Riyadh-11451, KSA*
[3]*Department of Chemistry, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, KSA.*
[4]*Department of Zoology, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, KSA.*

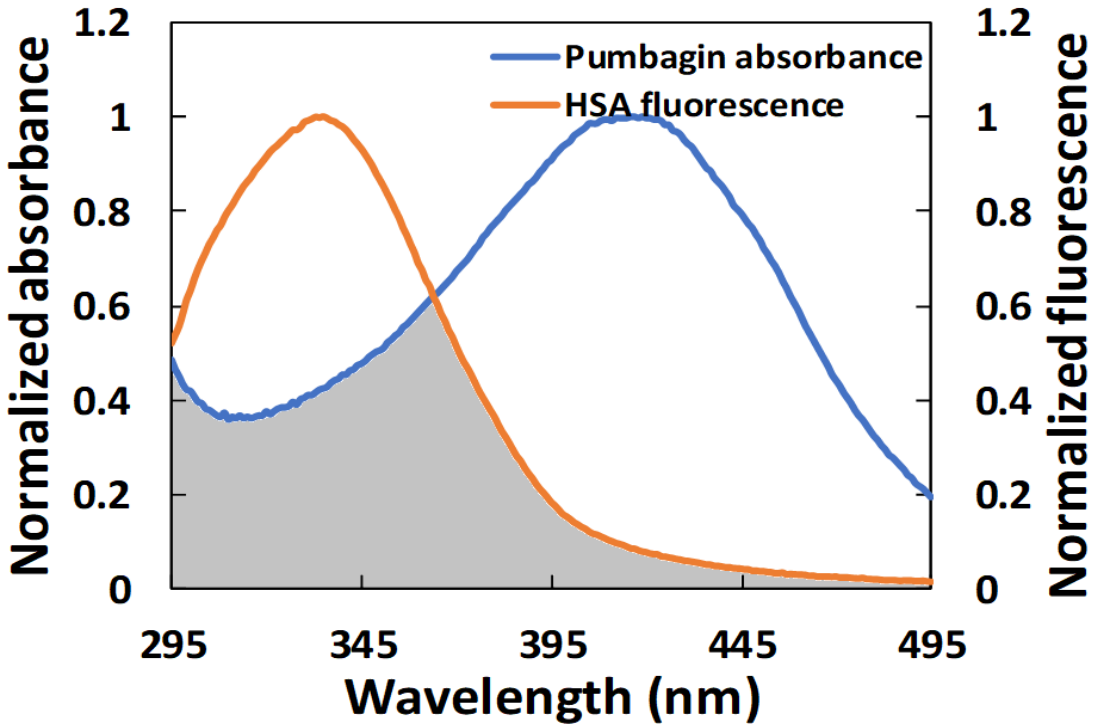
Corresponding author

Rais Ahmad Khan
krais@ksu.edu.sa (Khan, RA)
Department of Chemistry,
College of Science
King Saud University
P.O. Box 2455, Riyadh 11451
KSA.

Supplementary Figures



Supplementary Fig S1. Three-dimensional fluorescence spectra of (A) HSA (B) HSA-plumbagin complex.



Supplementary Fig S2. Spectral overlap of the fluorescence spectrum of HSA and absorption spectrum of plumbagin.

Supplementary Tables

Supplementary Table S1. α-helical content of HSA in the absence and presence of plumbagin.

Molar ratio ([HSA]/[plumbagin])	MRE_{208nm}	% α-helix
1:0	-20818.19	57.99
1:1	-18608.64	50.37
1:2	-17716.28	47.29

Supplementary Table S2. Förster resonance energy transfer data obtained from the spectral overlap of HSA and plumbagin.

Parameters	Values
Energy transfer efficiency (E)	29.04%
r	2.27 nm
Critical distance (R_0)	1.96 nm
Spectral overlap (J)	2.64×10^{-15} cm^3 L/mol

Supplementary Table S3. Changes in accessible surface area (ΔASA) in $Å^2$ for the HSA residues interacting with plumbagin.

S. No.	Residues	ASA ($Å^2$) in HSA	ASA ($Å^2$) in HSA–plumbagin complex	ΔASA ($Å^2$)	Domain
1.	Lys199	28.861	10.555	18.306	IIA
2.	Arg222	31.178	19.248	11.93	IIA
3.	Leu238	30.529	0.454	30.075	IIA
4.	Arg257	15.368	5.231	10.137	IIA
5.	Leu260	15.548	4.653	10.895	IIA
6.	Ile290	12.978	0	12.978	IIA
7.	Ala291	40.991	7.57	33.421	IIA