

# **Interaction of different prototropic species of an anticancer drug Ellipticine with HSA and IgG proteins: multispectroscopic and molecular modeling studies**

**Raina Thakur, Anupam Das, Vandna Sharma, Chandan Adhikari, Kalyan S Ghosh,\* and Anjan Chakraborty\***

**Author for correspondence:**

Dr. Anjan Chakraborty  
Department of Chemistry,  
Indian Institute of Technology Indore  
IET, M-Block, Indore 452017  
Email: [anjanc@iiti.ac.in](mailto:anjanc@iiti.ac.in)  
Fax: +91(0)731-2366382  
Tel: +91(0)731-2438706

Dr. Kalyan S. Ghosh  
Department of Chemistry,  
National Institute of Technology Hamirpur  
Himachal Pradesh 177005  
E-mail: [kalyan@nith.ac.in](mailto:kalyan@nith.ac.in)  
Fax: +91-1972-223834  
Tel: +91-1972-254104

## Supporting Information

**Table S1.** Distances (in Å) between interacting residues of HSA with the ligand

HSA residue	Distance
Lys 414 N	6.25 (N <sub>a</sub> )
Arg 410 N	10.72 (N <sub>b</sub> )
Arg 410 Nδ	9.63 (N <sub>a</sub> )
Lys 414 Nε	8.15 (N <sub>a</sub> )
Ser 489 O	10.82 (N <sub>a</sub> )

**Table S2.** Changes in accessible surface area of the amino acid residues of HSA on interaction with ellipticine

HSA residue	ASA (uncomplexed) (Å <sup>2</sup> )	ASA (protein-inhibitor complex) (Å <sup>2</sup> )	ΔASA (Å <sup>2</sup> )
Arg 410	71.25	50.09	21.16
Lys 413	42.62	1.72	40.9
Lys 414	13.38	6	7.38
Glu 492	120.56	100.64	19.92
Val 493	62.01	30.49	31.52
Lys 538	200.32	178.64	21.68
Thr 540	21.97	5.23	16.74
Lys 541	164.54	139.17	25.37

**Table S3.** Changes in accessible surface area of the amino acid residues of F<sub>ab</sub> region of IgG protein on interaction with ellipticine

Residues of F <sub>ab</sub> part	ASA of F <sub>ab</sub> residues uncomplexed (Å <sup>2</sup> )	ASA of F <sub>ab</sub> part in IgG ligand complex (Å <sup>2</sup> )
Phe 83	34.5	0
Ala 84	9.75	0
Leu 85	48.58	21.39
Arg 106	89.27	39.37
Gln 166	36.22	0
Asp 167	50.58	4.69
Ser 168	101.71	10.9

**Table S4.** Changes in accessible surface area of the amino acid residues of F<sub>c</sub> region of IgG protein on interaction with ellipticine

Residues of F <sub>c</sub> region of IgG protein	ASA (uncomplexed) (Å <sup>2</sup> )	ASA (protein-ligand complex) (Å <sup>2</sup> )
Ile 377	16.76	1.93
Ala 378	9.04	0.3
Val 379	14.76	0.4
Tyr 391	57.05	20.27
Thr 393	53.81	6.38
Thr 394	61.88	24.55
Pro 395	51.46	16.22
Leu 406	3.68	0.02

**Table S5.** Lifetime components and normalized amplitudes of lifetime components and average lifetime of ellipticine in presence of HSA at 440 nm.<sup>#</sup>

Conc. of HSA ( $\times 10^6$ M)	$a_1$	$a_2$	$\tau_1$ (ns)	$\tau_2$ (ns)	$\langle \tau \rangle$ (ns)
0	0.84	0.16	0.42	4.50	1.1
0.049	0.83	0.17	0.87	6.50	1.82
0.099	0.83	0.17	1.10	7.48	2.18
0.196	0.78	0.22	1.16	12.38	3.63
0.43	0.73	0.27	1.28	14.46	4.83
0.61	0.67	0.33	1.59	16.13	6.38
1	0.64	0.36	2.00	16.55	7.23
3	0.61	0.39	2.18	15.09	7.21
5	0.61	0.39	2.21	14.24	6.90
7	0.61	0.39	2.16	13.90	6.73
10	0.61	0.39	2.56	14.42	7.18

<sup>#</sup> Error in measurement is around 5-7%.

**Table S6A.** Lifetime components, normalized amplitudes of lifetime components and average lifetime of ellipticine in presence of native and heat denatured IgG at 540 nm. <sup>#</sup>

**Native IgG**

Conc. of IgG ( $\times 10^6$ M)	$a_1$	$a_2$	$\tau_1$ (ns)	$\tau_2$ (ns)	$\langle \tau \rangle$ (ns)
0	0.84	0.16	1.80	5.80	2.44
0.025	0.82	0.18	1.81	6.00	2.56
0.05	0.85	0.15	1.80	6.20	2.46
0.1	0.82	0.18	1.81	6.62	2.67
0.2	0.79	0.21	1.81	7.73	3.00
0.3	0.78	0.22	1.82	8.00	3.19
0.4	0.76	0.24	1.80	9.40	3.62
0.5	0.74	0.26	1.83	9.40	3.80
0.6	0.70	0.30	1.81	9.93	4.25
0.7	0.70	0.30	1.84	10.12	4.32
0.8	0.66	0.34	1.81	10.83	4.88
0.9	0.65	0.35	1.85	11.11	5.1
1.0	0.60	0.40	1.84	11.39	5.66
2.0	0.58	0.42	1.84	11.87	6.00
3.0	0.50	0.50	1.86	12.08	6.97
4.0	0.48	0.52	1.86	12.63	7.46
5.0	0.46	0.54	1.86	12.25	7.47
7.0	0.46	0.54	1.87	12.45	7.58
10.0	0.46	0.54	1.87	12.45	7.58

<b>Heat denatured IgG</b>					
<b>Conc. of IgG (<math>\times 10^6</math>M)</b>	<b><math>a_1</math></b>	<b><math>a_2</math></b>	<b><math>\tau_1</math> (ns)</b>	<b><math>\tau_2</math> (ns)</b>	<b><math>\langle \tau \rangle</math> (ns)</b>
0	0.84	0.16	1.8	5.8	2.44
0.025	0.81	0.19	1.57	6.52	2.51
0.05	0.78	0.22	1.43	6.87	2.63
0.1	0.76	0.24	1.45	7.15	2.82
0.2	0.75	0.25	1.42	7.36	2.90
0.4	0.74	0.26	1.41	7.60	3.0
0.6	0.73	0.27	1.35	8.00	3.16
0.8	0.73	0.27	1.35	8.61	3.31
1.0	0.73	0.27	1.41	9.44	3.58
2.0	0.74	0.26	1.49	10.28	3.77
3.0	0.73	0.27	1.53	11.32	4.17
5.0	0.70	0.3	1.62	12.36	4.84
7.0	0.69	0.31	1.64	12.39	4.97
10.0	0.68	0.32	1.58	12.50	5.10

# Error in measurement is around 5-7%.

**Table S6B.** Lifetime components, normalized amplitudes of lifetime components and average lifetime of ellipticine in presence of native and heat denatured IgG at 440 nm. #

<b>Native IgG</b>					
<b>Conc. of IgG (<math>\times 10^6</math>M)</b>	<b><math>a_1</math></b>	<b><math>a_2</math></b>	<b><math>\tau_1</math> (ns)</b>	<b><math>\tau_2</math> (ns)</b>	<b><math>\langle \tau \rangle</math> (ns)</b>
0	0.84	0.16	0.42	4.50	1.10
0.025	0.80	0.20	0.40	5.00	1.32
0.05	0.80	0.20	0.42	5.60	1.45
0.1	0.78	0.22	0.42	5.75	1.59
0.2	0.83	0.17	0.83	5.80	1.67
0.4	0.80	0.20	0.84	5.80	1.83
0.5	0.785	0.225	0.86	6.00	2.00
0.7	0.77	0.23	1.00	6.20	2.21
0.8	0.76	0.24	0.97	6.48	2.29
1.0	0.75	0.25	0.99	6.60	2.39
2.0	0.74	0.26	1.12	6.86	2.61
3.0	0.74	0.26	1.10	7.20	2.69
5.0	0.74	0.26	1.20	7.91	2.94
7.0	0.74	0.26	1.19	8.19	3.00
10.0	0.74	0.26	1.10	8.33	2.98

  

<b>Heat denatured IgG</b>					
<b>Conc. of IgG (<math>\times 10^6</math>M)</b>	<b><math>a_1</math></b>	<b><math>a_2</math></b>	<b><math>\tau_1</math> (ns)</b>	<b><math>\tau_2</math> (ns)</b>	<b><math>\langle \tau \rangle</math> (ns)</b>
0	0.84	0.16	0.42	4.50	1.10
0.025	0.80	0.20	0.55	5.2	1.50
0.05	0.78	0.22	0.64	6.00	1.83
0.1	0.77	0.23	0.64	6.44	1.97

0.2	0.76	0.24	0.76	6.66	2.17
0.4	0.76	0.24	0.833	6.94	2.30
0.6	0.75	0.25	0.97	7.64	2.64
0.8	0.73	0.27	1.11	8.00	2.98
1.0	0.71	0.29	1.25	8.47	3.34
2.0	0.68	0.32	1.38	8.75	3.74
3.0	0.67	0.33	1.52	9.00	3.99
5.0	0.66	0.34	1.59	9.00	4.12
7.0	0.62	0.38	1.66	9.10	4.50
10.0	0.60	0.40	1.66	9.50	4.80

# Error in measurement is around 5-7%.