

Erratum

Erratum to “The interaction of silibinin with human serum albumin: A spectroscopic investigation”

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Natural silibinin being a mixture of silibinin A and silibinin B, we include the corrected structures. The description of chirality in the paper is hereby modified. The experimental results obtained are with the compound purchased from Sigma (Catalogue No. S0417) (Fig. E1).

The docking studies in the paper are for silibinin A. Table E1 shows a comparison for the residues involved in the interaction as obtained from docking studies for silibinin A and B.

Stereoview of the docking pose of HSA and silibinin B, residues within hydrogen bonding distance of silibinin are marked.

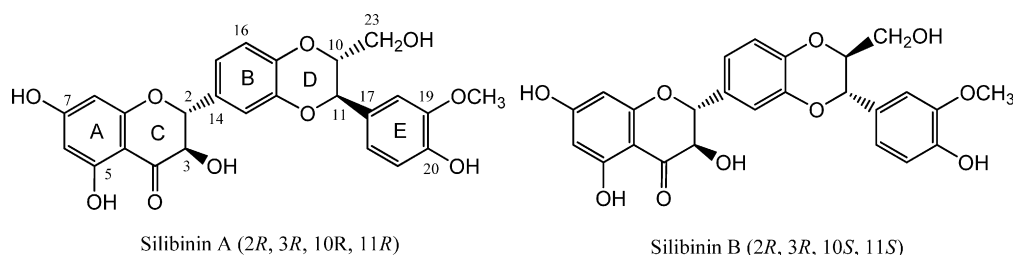


Fig. E1. Silibinin A, (2*R*,3*R*)-2-[(2*R*,3*R*)-2,3-dihydro-3-(4-hydroxy-3-methoxyphenyl)-2-(hydroxymethyl)-1,4-benzodioxin-6-yl]-2,3-dihydro-3,5,7-trihydroxy-4*H*-1-benzopyran-4-one and silibinin B (2*R*,3*R*)-2-[(2*S*,3*S*)-2,3-dihydro-3-(4-hydroxy-3-methoxyphenyl)-2-(hydroxymethyl)-1,4-benzodioxin-6-yl]-2,3-dihydro-3,5,7-trihydroxy-4*H*-1-benzopyran-4-one.

Table E1

Accessible surface areas (ASA) of HSA and the HSA–silibinin docked complex.

Residue	ASA (Å ²) (HSA)	ASA (Å ²) (HSA–silibinin A)	ASA (Å ²) (HSA–silibinin B)	ΔASA (Å ²) (silibinin A)	ΔASA (Å ²) (silibinin B)	Location
Lys 195	91.36	39.60	30.52	51.76	60.84	Ib-h4
Lys 199	32.01	6.58	28.47	25.43	3.54	Ila-h1
Trp 214	61.74	25.42	38.48	36.32	23.26	Ila-h2
Arg 218	41.96	18.94	13.08	23.02	28.88	Ila-h2
Arg 222	37.12	9.39	18.78	27.73	18.34	Ila-h2
Leu 238	30.64	4.39	30.64	26.25	0.00	Ila-h3
Ala 291	36.99	0.00	36.99	36.99	0.00	Ila-h6
Asp 451	30.24	2.13	12.67	28.11	17.57	IIla-h4

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