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Spectroscopic and molecular docking elucidation to binding characteristics of bovine serum albumin with bupropion an aminoketone-medication for nicotine addiction

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RESEARCH ARTICLE

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KEYWORDS

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ABSTRACT

One of the highly soluble protein presents in circulatory system of bovine body is bovine serum albumin (BSA). Bupropion hydrochloride (BRN) served to treat prime smoking cessation and disorder due to depressive. BRN binding to BSA was studied by molecular docking and lots of spectroscopic (UV-vis, emission, synchronous, 3D fluorescence, CD and FT-IR) methods at pH = 7.40. Static quenching with strong binding was obtained for BSA-BRN system by forming complex. Secondary structures, conformations and microenvironments of BSA were altered after BRN interaction. Distance between BRN and BSA was also achieved. Biologically active metal ions (Cu^{2+}, Ca^{2+}, Mg^{2+}, Fe^{2+} and Zn^{2+}) were also influenced on the BSA-BRN complex. Bonds of hydrogen and Van der Waals were major binding forces to stabilize BSA-BRN complex at site I (IIA) of BSA. Hence, binding of BRN to transport protein (BSA) is of prominent importance and these findings could be helpful for BRN pharmacology and potential clinical research.

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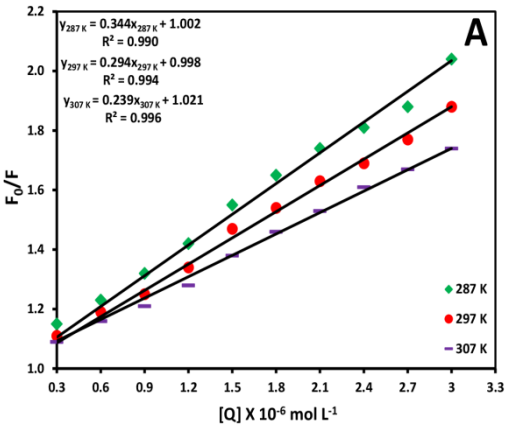
SUPPLEMENTARY MATERIALS



http://dx.doi.org/10.5155/eurjchem.10.2.146-155.1845

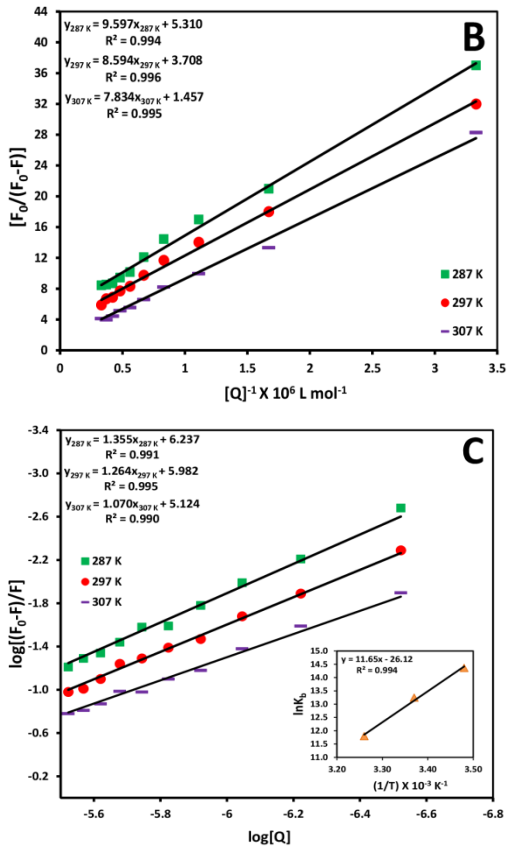


Figure S1. Plots for BSA–BRN system: (A), (B), (C) and inset of (C) are Stern-Volmer, Modified Stern-Volmer, $\log[(F_0 - F)/F]$ versus $\log[Q]$ and Van't Hoff, respectively at temperatures 287, 297 and 307 K.

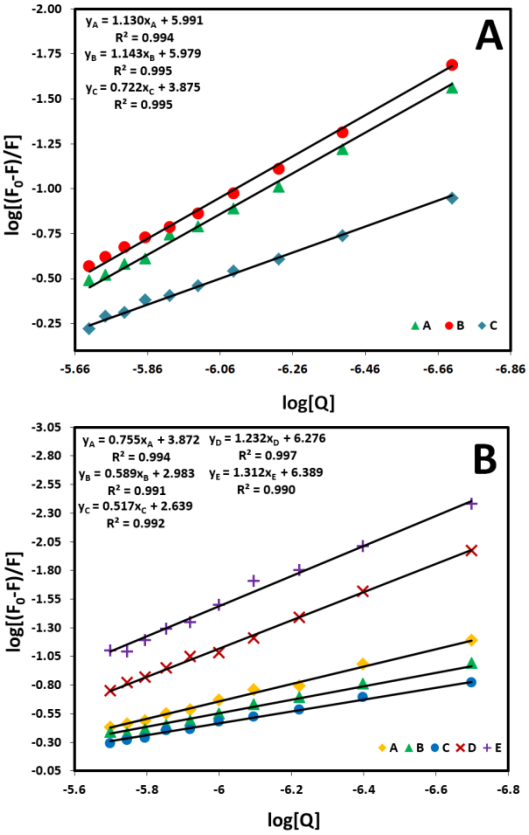


Figure S2. Plot of $\log[(F_0 - F)/F]$ adjacent to $\log[Q]$ for BSA-BRN system at 297 K: (A) site markers (A, B and C were digitoxin, ibuprofen and warfarin, respectively) and (B) metal ions (A, B, C, D and E were Mg^{2+}, Cu^{2+}, Zn^{2+}, Ca^{2+} and Fe^{2+}, respectively).

Table S1. Lamarckian Genetic Algorithm to BSA−BRN system at top ranked conformations by docking analysis *.

Rank	Run	ΔG (KJ mol^{-1})	$E_{inter-mol}$ (KJ mol^{-1})	$E_{vdw+HB+desol}$ (KJ mol^{-1})	E_{Elec} (KJ mol^{-1})
1	41	−30.12	−35.10	−35.02	−0.083
2	25	−30.04	−35.02	−34.93	−0.083
3	76	−29.79	−34.76	−34.43	−0.334
4	31	−29.66	−34.68	−34.30	−0.334
5	69	−29.53	−34.51	−34.18	−0.334

* ΔG is the binding free energy, $E_{inter-mol}$is the intermolecular interaction energy; sum of vander Waals energy, hydrogen bonding energy, desolvation free energy and electrostatic energy, $E_{vdw+HB+desol}$ is the sum of Vander Waals energy, hydrogen bonding energy and desolvation free energyE_{Elec} is the electrostatic energy.

Table S2. Presence of metal ions and site markers affects the BSA-BRN system at 297 K *.

System	K_b (L mol^{-1})
BSA−BRN	$9.59\pm0.03 \times 10^5$
BSA−BRN −warfarin	$7.49\pm0.08 \times 10^3$
BSA−BRN −ibuprofen	$9.53\pm0.04 \times 10^5$
BSA−BRN −digitoxin	$9.79\pm0.06 \times 10^5$
BSA−BRN− Cu^{2+}	$9.62\pm0.07 \times 10^2$
BSA−BRN − Ca^{2+}	$1.89\pm0.01 \times 10^6$
BSA−BRN − Mg^{2+}	$7.45\pm0.09 \times 10^3$
BSA−BRN − Fe^{2+}	$2.45\pm0.03 \times 10^6$
BSA−BRN − Zn^{2+}	$4.36\pm0.05 \times 10^2$

* K_b is binding constant.