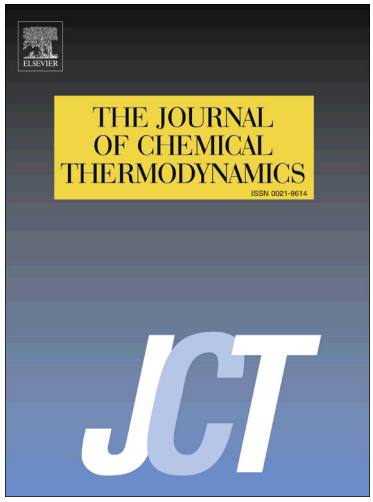

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Samima Khatun, Riyazuddeen, Shama Yasmeen, Amarjeet Kumar, Naidu Subbarao

PII: S0021-9614(18)30152-6
DOI: https://doi.org/10.1016/j.jct.2018.03.004
Reference: YJCHT 5349

To appear in: *J. Chem. Thermodynamics*

Received Date: 31 October 2017
Revised Date: 16 February 2018
Accepted Date: 5 March 2018

Please cite this article as: S. Khatun, Riyazuddeen, S. Yasmeen, A. Kumar, N. Subbarao, Calorimetric, spectroscopic and molecular modelling insight into the interaction of Gallic acid with bovine serum albumin, *J. Chem. Thermodynamics* (2018), doi: https://doi.org/10.1016/j.jct.2018.03.004

Calorimetric, spectroscopic and molecular modelling insight into the interaction of Gallic acid with bovine serum albumin

Samima Khatun[a], Riyazuddeen[a]*, Shama Yasmeen[a], Amarjeet Kumar[b], Naidu Subbarao[b]

[a]Department of Chemistry, Aligarh Muslim University, Aligarh, 202002, U.P, India
[b]School of Computational and Integrative Science, Jawaharlal Nehru University, New Delhi, India

*Corresponding Author
Email: rz1@rediffmail.com

ABSTRACT

Gallic acid (GA), a naturally occurring plant phenolic acid effectively used as antioxidant, anti-carcinogenic, antifungal, anti-inflammatory and in anti-human rhinovirus activities. The present study reports *in vitro* interaction studies of Gallic acid (GA) with bovine serum albumin (BSA) by using isothermal titration calorimetric (ITC), fluorescence, circular dichroism (CD) and molecular modelling studies. The association constant (K_a), enthalpy change (ΔH^o), entropy change (ΔS^o) and Gibbs energy change (ΔG^o) were obtained from ITC. The fluorescence results indicate that there was static quenching mechanism in the interactions of GA with BSA. The Synchronous and 3D fluorescence spectroscopy confirms conformational alteration of BSA in presence of GA which is further supported by CD. Molecular docking analysis highlighted that GA binds at Sudlow site I of BSA which also confirmed from site probe experiments. In addition, the molecular dynamics (MD) simulation study of BSA and BSA-GA complex shows that binding of GA at site I of BSA is stable and the binding Gibbs energies from the molecular mechanics/Poisson-Boltzmann surface area method showed that van der Waals forces are the predominant intermolecular forces. This study reflects greater pharmacological significance of GA and highlights its importance in the clinical medicine.

Keywords: Bovine serum albumin; Gallic acid; Isothermal titration calorimetry; Spectroscopy; molecular docking; molecular dynamic simulation.