

Interaction of levothyroxine with bovine serum albumin

Nicoleta Sandu^{1*}, Claudia G. Chilom¹, Melinda David², Monica Florescu², Aurel I. Popescu¹

¹Department of Electricity, Solid Physics and Biophysics, Faculty of Physics, University of Bucharest, Măgurele, Romania, Postal address: Str. Atomistilor no. 405, CP MG - 11, Bucuresti-Magurele, RO - 077125, Romania;

*Doctoral School of the Faculty of Physics, University of Bucharest

²Department of Fundamental, Prophylactic and Clinical Disciplines, Faculty of Medicine, Transilvania University of Brasov, Brasov, Romania, Str. Universitatii no. 1, Building C, room CI30, 500068 Brasov, Romania

e-mail: nicoleta.sandu@drd.unibuc.ro

ABSTRACT

Research motivation. Levothyroxine (LT4), $C_{15}H_{11}L_4NO_4$, is a synthetic form of thyroid hormone, tetraiodothyronine (T4), used to treat thyroid hormone deficiency by suppressing thyroid stimulating hormone (TSH) [Colucci *et al.*, 2013; Glivic *et al.*, 2015].

Understanding the mechanisms of interaction of LT4 with biological molecules, but also with some molecules that contain active principles, can bring benefits in the treatment of cancer, but also in other diseases. The aim of this study is to characterize these interaction mechanisms, in order to make new contributions in the medical field.

Methodology. At the moment of the study, characterization of interactions between LT4 and bovine serum albumin (BSA) was performed using experimental methods (UV-VIS spectroscopy, Fourier-transform infrared spectroscopy, Förster resonance energy transfer, Surface plasmon resonance) and computational (molecular docking) [Chilom *et al.*, 2018, Sandu *et al.*, 2020].

Results. UV-Vis spectrometry was used to determine the optimal pH value of LT4 in HEPES buffer. Fluorescence experiments have shown that LT4 interacts with BSA mainly through a static mechanism and affects protein conformation at the binding site. The results obtained in the molecular docking process, in the absence of the solvent, suggest the binding of LT4 to another BSA site, with a lower binding affinity.

Conclusions and Perspectives. The investigation of the interaction of LT4 with BSA has led to results that may have applicability in the medical field. In the future, we intend to investigate the action of LT4 on normal and tumour cell lines, to determine its effect on cell viability and the effects of biocompatibility / toxicity.

Keywords: Physics, LT4, BSA, UV – Vis, SPR

Field: Physics

Section: Elaboration of the doctoral thesis

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