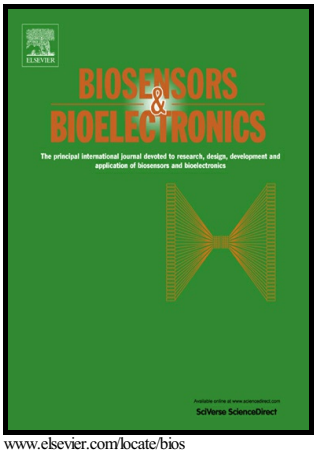

www.elsevier.com/locate/bios

Theoretical and experimental study for the biomimetic recognition of levothyroxine hormone on magnetic molecularly imprinted polymer

Silio Lima Moura, Laura Martinez Fajardo, Leonardo dos Anjos Cunha, Maria Del Pilar Taboada Sotomayor, Francisco Bolivar Correto Machado, Luiz Fernando de Araújo Ferrão, Maria Isabel Pividori

PII: S0956-5663(18)30041-1
DOI: https://doi.org/10.1016/j.bios.2018.01.028
Reference: BIOS10221

To appear in: *Biosensors and Bioelectronic*

Received date: 10 November 2017
Revised date: 9 January 2018
Accepted date: 13 January 2018

Cite this article as: Silio Lima Moura, Laura Martinez Fajardo, Leonardo dos Anjos Cunha, Maria Del Pilar Taboada Sotomayor, Francisco Bolivar Correto Machado, Luiz Fernando de Araújo Ferrão and Maria Isabel Pividori, Theoretical and experimental study for the biomimetic recognition of levothyroxine hormone on magnetic molecularly imprinted polymer, *Biosensors and Bioelectronic,* https://doi.org/10.1016/j.bios.2018.01.028

Theoretical and experimental study for the biomimetic recognition of levothyroxine hormone on magnetic molecularly imprinted polymer

Silio Lima Moura[a1], Laura Martinez Fajardo[a1], Leonardo dos Anjos Cunha[b], Maria Del Pilar Taboada Sotomayor[c], Francisco Bolivar Correto Machado[b], Luiz Fernando de Araújo Ferrão[b,*], Maria Isabel Pividori[a,*]

[a]Grup de Sensors i Biosensors, Departament de Química, Universitat Autònoma de Barcelona, 08193, Bellaterra, Spain
[b]Instituto Tecnológico de Aeronáutica, Departamento de Química, São José dos Campos, 12228-900, São Paulo, Brazil
[c]Instituto de Química, Departmento de Química Analítica, Universidade Estadual de São Paulo (UNESP), 14801-970, Araraquara, São Paulo, Brazil

ferrao@ita.br

isabel.pividori@uab.cat

***Corresponding authors:**

Abstract

This study addresses the rational design of a magnetic molecularly imprinted polymer (magnetic-MIP) for the selective recognition of the hormone levothyroxine. The theoretical study was carried out by the density functional theory (DFT) computations considering dispersion interaction energies, and using the D2 Grimme's correction. The B97-D/def2-SV(P)/PCM method is used not only for studying the structure of the template the and monomer-monomer interactions, but also to assess the stoichiometry, noncovalent binding energies, solvation effects, and thermodynamics properties such as binding energy. Among the 13 monomers studied *in silico*, itaconic acid is the most suitable according to the thermodynamic values. In order to assess the efficiency of the computational study, three different magnetic-MIPs based on itaconic acid, acrylic acid and acrylamide were synthesized and experimentally compared. The theoretical results are in agreement with experimental binding studies based on laser confocal microscopy, magneto-actuated immunoassay and electrochemical sensing. Furthermore, and for the first time, the direct electrochemical sensing of L-thyroxine preconcentrated on magnetic-MIP was successfully performed on magneto-actuated electrodes within 30 min with a limit of detection of as low as 0.0356 ng mL^{-1} which cover the clinical range of total L-thyroxine. Finally, the main analytical features were compared with the gold standard method based on commercial competitive immunoassays. This work provides a thoughtful strategy for magnetic molecularly imprinted polymer design,

[1] These authors contributed equally to this work