

Accepted Manuscript

Title: *In silico* investigation of propofol binding sites in human serum albumin using explicit and implicit solvation models

Authors: Sergey Shityakov, Norbert Roewer, Carola Förster, Jens-Albert Broscheit



PII: S1476-9271(17)30350-X
DOI: <http://dx.doi.org/doi:10.1016/j.compbiolchem.2017.06.004>
Reference: CBAC 6702

To appear in: *Computational Biology and Chemistry*

Received date: 23-5-2017
Revised date: 24-6-2017
Accepted date: 27-6-2017

Please cite this article as: Shityakov, Sergey, Roewer, Norbert, Förster, Carola, Broscheit, Jens-Albert, In silico investigation of propofol binding sites in human serum albumin using explicit and implicit solvation models. *Computational Biology and Chemistry* <http://dx.doi.org/10.1016/j.compbiolchem.2017.06.004>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

***In silico* investigation of propofol binding sites in human serum albumin using explicit and implicit solvation models**

Sergey Shityakov^{1,*}, Norbert Roewer^{1,2}, Carola Förster¹, and Jens-Albert Broscheit^{1,2}

¹Department of Anesthesia and Critical Care, University of Würzburg, 97080 Würzburg, Germany

²Sapiotec Ltd., 97078 Würzburg, Germany

* Author to whom correspondence should be addressed:

Sergey Shityakov

Department of Anesthesia and Critical Care

University of Würzburg

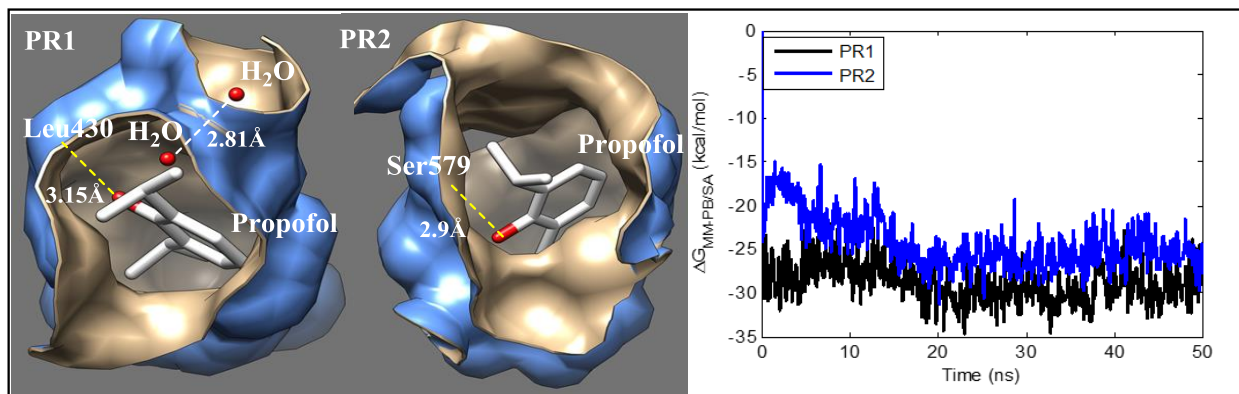
97080 Würzburg, Germany

E-Mail: Shityakov_S@ukw.de

Tel: + 49 (931) 201 - 30016

Fax: + 49 (931) 201 - 30019

Graphical Abstract:



Download English Version:

<https://daneshyari.com/en/article/4752600>

Download Persian Version:

<https://daneshyari.com/article/4752600>

[Daneshyari.com](https://daneshyari.com)