## Accepted Manuscript

Title: Multiscale molecular dynamics simulations of lipid interactions with P-glycoprotein in a complex membrane

Authors: Laura Domicevica, Heidi Koldsø, Philip C. Biggin

PII:	S1093-3263(17)30247-4
DOI:	http://dx.doi.org/10.1016/j.jmgm.2017.09.002
Reference:	JMG 7018
To appear in:	Journal of Molecular Graphics and Modelling
Received date:	9-6-2017
Revised date:	29-8-2017
Accepted date:	1-9-2017

Please cite this article as: Laura Domicevica, Heidi Koldsø, Philip C.Biggin, Multiscale molecular dynamics simulations of lipid interactions with P-glycoprotein in a complex membrane, Journal of Molecular Graphics and Modellinghttp://dx.doi.org/10.1016/j.jmgm.2017.09.002

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.



## ACCEPTED MANUSCRIPT

## Multiscale molecular dynamics simulations of lipid interactions with P-glycoprotein in a complex membrane

Running Title: "P-glycoprotein in a complex membrane"

Laura Domicevica<sup>1</sup>, Heidi Koldsø<sup>1,‡</sup> and Philip C. Biggin<sup>1\*</sup>

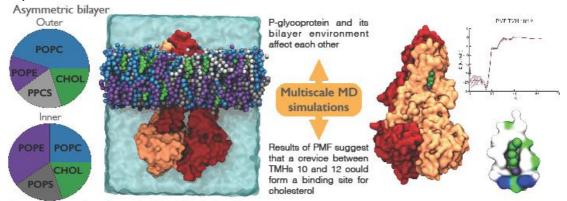
<sup>1</sup>Structural Bioinformatics and Computational Biochemistry, Department of Biochemistry, University of Oxford, South Parks Road, Oxford, OX1 3QU, United Kingdom.

<sup>‡</sup>Present address: D. E. Shaw Research, 120 West 45th Street, 39th Floor, New York, New York 10036, United States of America.

\*To whom correspondence should be addressed.

Email: philip.biggin@bioch.ox.ac.uk

Tel. +44 1865 613305



Graphical abstract

Composition taken from the blood brain barrier

Download English Version:

## https://daneshyari.com/en/article/4953154

Download Persian Version:

https://daneshyari.com/article/4953154

Daneshyari.com