Exploring the Local Elastic Properties of Bilayer Membranes Using Molecular Dynamics Simulations - DTU Orbit (08/11/2017)

Exploring the Local Elastic Properties of Bilayer Membranes Using Molecular Dynamics Simulations

Membrane mechanical elastic properties regulate a variety of cellular processes involving local membrane deformation, such as ion channel function and vesicle fusion. In this work, we used molecular dynamics simulations to estimate the local elastic properties of a membrane. For this, we calculated the energy needed to extract a DOPE lipid molecule, modified with a linker chain, from a POPC bilayer membrane using the umbrella sampling technique. Although the extraction energy entails several contributions related not only to elastic deformation but also to solvation, careful analysis of the potential of mean force (PMF) allowed us to dissect the elastic contribution. With this information, we calculated an effective linear spring constant of 44 +/- 4 kJ.nm^{-2}.mol^{-1} for the DOPC membrane, in agreement with experimental estimates. The membrane deformation profile was determined independently during the stretching process in molecular detail, allowing us to fit this profile to a previously proposed continuum elastic model. Through this approach, we calculated an effective membrane spring constant of 42 kJ^{-2}.mol^{-1}, which is in good agreement with the PMF calculation. Furthermore, the solvation energy we derived from the data is shown to match the solvation energy estimated from critical micelle formation constants. This methodology can be used to determine how changes in lipid composition or the presence of membrane modifiers can affect the elastic properties of a membrane at a local level.

General information

State: Published
Organisations: Physical and Biophysical Chemistry, Department of Chemistry, Universidad de los Andes
Authors: Pieffet, G. (Ekstern), Botero, A. (Ekstern), Peters, G. H. (Intern), Forero-Shelton, M. (Ekstern), Leidy, C. (Ekstern)
Number of pages: 9
Pages: 12883-12891
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Physical Chemistry B
Volume: 118
Issue number: 45
ISSN (Print): 1520-6106
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.03 SJR 1.348 SNIP 1.02
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.367 SNIP 1.096 CiteScore 3.25
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.44 SNIP 1.14 CiteScore 3.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.494 SNIP 1.2 CiteScore 3.53
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.92 SNIP 1.251 CiteScore 3.66
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.78 SNIP 1.226 CiteScore 3.62
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.849 SNIP 1.214
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1

Scopus rating (2009): SJR 2.232 SNIP 1.349
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.543 SNIP 1.381
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.346 SNIP 1.282
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.369 SNIP 1.415
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.275 SNIP 1.474
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.148 SNIP 1.511
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.034 SNIP 1.47
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.118 SNIP 1.496
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.053 SNIP 1.508
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.145 SNIP 1.527
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.713 SNIP 1.8
Original language: English
DOIs:
10.1021/jp504427a
Source: FindIt
Source-ID: 272738504
Publication: Research - peer-review › Journal article – Annual report year: 2015