# Universidade de São Paulo
# Instituto de Física de São Carlos

# Semana Integrada do Instituto de Física de São Carlos

**13ª edição**

# Livro de Resumos

São Carlos
2023

Ficha catalográfica elaborada pelo Serviço de Informação do IFSC

Semana Integrada do Instituto de Física de São Carlos
(13: 21-25 ago.: 2023: São Carlos, SP.)
Livro de resumos da XIII Semana Integrada do Instituto de Física de São Carlos – Universidade de São Paulo / Organizado por Adonai Hilário da Silva [et al.]. São Carlos: IFSC, 2023.
358p.

Texto em português.
1.Física. I. Silva, Adonai Hilário da, org. II. Título.

ISSN: 2965-7679

# PG164

# Molecular dynamics simulations of drug interactions with cell membrane models

OLIVEIRA JUNIOR., Osvaldo Novais de[1]; ZAPATA, Juan Carlos Burbano[1]; MOURA, André Farias de[2]

juan.burbano@ifsc.usp.br

[1]Instituto de Física de São Carlos - USP; [2]Departamento de Química - UFSCar

Levofloxacin is a broad-spectrum antibiotic used to fight infections in the respiratory system,whose action in topical administration (via inhalation) depends on molecular-level interactions with the alveolar membrane. (1) Here, we investigate the interaction between levofloxacin and Langmuir monolayers mimicking the lung surfactant. The possible conformations and hydrophilicity of levofloxacin upon interacting with water were determined using optimized coarse-grained (CG) MARTINI forcefield parameters for the zwitterionic levofloxacin of bonded and nonbonded parameters. (2) The CG structure for levofloxacin was compatible with that obtained in atomistic simulations, yielding similar radii of gyration and octanol-water partition coefficient. The influence of levofloxacin on a Langmuir monolayer of hydrated dipalmitoylphosphatidylcholine (DPPC), one of the main components of lung surfactant, was studied with molecular dynamics (MD) simulations. Levofloxacin induces an increase in pressure for the phase transition in surface pressure-area isotherms, consistent with experimental results. (3) It also causes an increase in surface pressure and displacement to larger areas, with monolayer expansion and stability. Levofloxacin molecules are accumulated in the DPPC-water interface, being forced to the headgroup region upon compression as verified in the charge density and DPPC-levofloxacin energy distributions. The presence of levofloxacin has little effect on the DPPC-water interaction, i.e. it does not affect the total value of the Coulomb and LJ energies. These findings may provide insights into efficient ways for topical medication with this drug.

**Palavras-chave:** Levofloxacin. Langmuir DPPC monolayer model. Surface pressure-area isotherm.

**Agência de fomento:** CNPq (141000/2019-8)

**Referências:**

1 EZELARAB, H. A. A. *et al*. Recent updates of fluoroquinolones as antibacterial agents. **Archid der Pharmazie**, v. 351, n. 9, p. e1800141, 2018. DOI: 10.1002/ardp.201800141.

2 MARRINK, S. J.; DE VRIES, A. H.; MARK, A. E. Coarse grained model for semiquantitative lipid simulations. **Journal of Physical Chemistry B**, v. 108, n. 2, p. 750–760, 2004. DOI: 10.1021/jp036508g.

3 ORTIZ-COLLAZOS, S. *et al*. Interaction of levofloxacin with lung surfactant at the air-water interface. **Colloids Surfaces B** - biointerfaces, v. 158, p. 689–696, 2017. DOI: 10.1016/j.colsurfb.2017.07.066.