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An International Journal at the Interface Between Chemistry and Physics

Volume 122, 2024 - [Issue 21-22: Luis Rull, Jose Luis Abascal and the Spanish School of Statistical Mechanics](#)

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Rull-Abascal Special Issue for Statistical Physics in Spain (by invitation only)

Absorption of active pharmaceutical ingredients in a protein/lipid bilayer by dissipative particle dynamics

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Article: e2394624 | Received 03 May 2024, Accepted 12 Aug 2024, Published online: 27 Aug 2024

 Cite this article

 <https://doi.org/10.1080/00268976.2024.2394624>

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Abstract

Mesoscopic simulations are performed to study the absorption of eriodictyol and favipiravir for a charged protein inserted in a lipid bilayer. The dissipative particle dynamics (DPD) force field parameters of both compounds are obtained to approximate

