Journal of Mosaic of Autoimmunity
https://www.sciltp.com/journals/jmai

Short Communication

Supplementary Materials: The Ro60-Ro52 Complex as a New Player in Intracellular Humoral Immunity

Jesus Vicente de Julián-Ortiz [1,*], Federico V. Pallardó [2,3], Pilar González-Cabo [2,3], Salvador Blasco [4] and David Gimenez-Romero [5,*]

[1] Department of Physical Chemistry, Faculty of Pharmacy, University of Valencia, Av. Vicent Andrés Estellés 0, 46100 Valencia, Spain
[2] Department of Physiology, Faculty of Medicine and Dentistry, University of Valencia-INCLIVA, 46010 Valencia, Spain
[3] CIBER Rare Diseases (CIBERER), 46010 Valencia, Spain
[4] Department of Inorganic Chemistry, Faculty of Chemistry, University of Valencia, C/Doctor Moliner 50, 46100 Burjassot, Spain
[5] Department of Physical Chemistry, Faculty of Chemistry, University of Valencia, C/Doctor Moliner 50, 46100 Burjassot, Spain
* Correspondence: jesus.julian@uv.es (J.V.d.J.-O.); david.gimenez-romero@uv.es (D.G.-R.)

How To Cite: de Julián-Ortiz, J.V.; Pallardó, F.V.; González-Cabo, P.; et al. The Ro60-Ro52 Complex as a New Player in Intracellular Humoral Immunity. *Journal of Mosaic of Autoimmunity* **2025**, *1*, 2

Experimental Section: Computer Calculations

Initial structures were obtained from our previous research [1] and prepared for simulation. All simulations were carried with GROMACS 2024 [2] with the built-in CHARMM-27 [3] force field and TIP3P water model. NaCl was added to achieve electroneutrality and reach 0.1 M concentration. The box was sized so that it could accommodate enough room for pulling the chains apart in the y direction. Water molecules were restrained with LINCS [4,5]. Electrostatic were treated with PME [6]. After energy minimisation, a short NPT equilibration of 200ps was run. The NPT ensemble was done with velocity rescaling [7] and cell rescaling [8] for temperature and pressure control fixed at 300 K and 1 atm respectively. After the equilibration, a pull force of 2000 kJ/mol.nm^2 was applied to the center of mass of chains of Ro52 and center of mass of chain of Ro60 to force the separation of the two groups at a rate of 0.008 nm/ps during 1 ns in order to achieve a final separation of ca. 11.6 nm. This trajectory was divided into 55 frames of ca. 0.14 nm step. Each of the frames was equilibrated in an NPT ensemble for 200 ps with the umbrella potential on and then the production run was performed for 1 nm in the same conditions. The collection of production data was processed by the weighted histogram analysis [9] to produce the final results: ΔG = +359.65 kJ/mol for the process Ro60-Ro52 ⇔ Ro60 + Ro52.

An animation based on this Umbrella Sampling Molecular Dynamics simulation can be seen in the reference [10].

References

1. Rodríguez, L.; de Julián-Ortiz, J.V.; de la Rúa, F.; et al. Unveiling the Ro60-Ro52 Complex. *EXCLI J.* **2024**, *23*, 888–903.
2. Abraham, M.J.; Murtola, T.; Schulz, R.; et al. GROMACS: High performance molecular simulations through multi-level parallelism from laptops to supercomputers. *SoftwareX* **2015**, *1*, 19–25.
3. Bjelkmar, P.; Larsson, P.; Cuendet, M.A.; et al. Implementation of the CHARMM force field in GROMACS: Analysis of protein stability effects from correction maps, virtual interaction sites, and water models. *J. Chem. Theory Comput.* **2010**, *6*, 459–466.
4. Hess, B.; Bekker, H.; Berendsen, H.J.C.; et al. LINCS: A Linear Constraint Solver for molecular simulations. *J. Comput. Chem.* **1997**, *18*, 1463–1472.
5. Miyamoto, S.; Kollman, P.A. SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for Rigid Water Models. *J. Comput. Chem.* **1992**, *13*, 952–962.
6. Essmann, U.; Perera, L.; Berkowitz, M.L.; et al. A smooth particle mesh Ewald method. *J. Chem. Phys.* **1995**, *103*, 8577–8592.

7. Bussi, G.; Donadio, D.; Parrinello, M. Canonical sampling through velocity rescaling. *J. Chem. Phys.* **2007**, *126*, 014101.
8. Bernetti, M.; Bussi, G. Pressure control using stochastic cell rescaling. *J. Chem. Phys.* **2020**, *153*, 114107.
9. Hub, J.S.; de Groot, B.L.; van der Spoel, D. g_wham-A free weighted histogram analysis implementation including robust error and autocorrelation estimates. *J. Chem. Theory Comput.* **2010**, *6*, 3713–3720.
10. Available online: https://www.uv.es/jejuor/SLE/Umbrella%20Sampling%20Pull.mp4 (accessed on 14 January 2025).