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Jesús Ignacio Mendieta Moreno PhD. - Former Member First-principles Atomistic Simulation Techniques

Biographical Info

PhD. Universidad Autónoma de Madrid 2018.
Master degree in Biophysics, Universidad Autónoma de Madrid 2011.
Physics degree, Universidad Autónoma de Madrid 2010.

Research Interests

Biophysics.
DFT simulation.
MD simulations.
Computational Biology.
Structural Biology.

Relevant/Recent Publications

Mendieta-Moreno, J.I., Walker, R., Lewis, J., Gómez-Puertas, P., Mendieta, J. & Ortega, J, FIREBALL/AMBER: An efficient local-orbital DFT QM/MM method for biomolecular systems. Journal of Chemical Theory and Computation 10, 2185–2193, (2014). [URL]

Martín-García, F., Mendieta-Moreno, J.I., Marcos-Alcalde, I, Gómez-Puertas, P. & Mendieta, J, Simulation of catalytic water activation in mitochondrial F1-ATPase using a hybrid quantum mechanics/molecular mechanics approach: An alternative role for ß-Glu 188. Biochemistry 52, 959-966, (2013). [URL]

Martín-García, F., Salvarelli, E., Mendieta-Moreno, J.I., Vicente, M., Mingorance, J., Mendieta, J. & Gómez-Puertas, P, Molecular dynamics simulation of GTPase activity in polymers of the cell division protein FtsZ. FEBS Letters 586, 1236–1239, (2012). [URL]

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dynamics analysis of conformational change of paramyxovirus F protein during the initial steps of membrane fusion. Biochemical and Biophysical Research Communications 420, 42-47, (2012). [URL]
Martín-García, F., Mendieta-Moreno, J.I., López-Viñas, E., Gómez-Puertas, P. & Mendieta, J, The Role of Gln(61) in HRas GTP Hydrolysis: A Quantum Mechanics/Molecular Mechanics Study. Biophysical Journal 102, 152-157, (2012). [URL]