

# Genome Informatics

## Simulation of photosystem II dynamics in the thylakoid membrane



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Photosystem II (PSII) is a key player in photosynthesis. The dynamics of PSII are however difficult to study experimentally, due to the time and length scales involved. To overcome this barrier we performed using the Martini force field<sup>1,2</sup>, coarse grained molecular dynamics simulations of Photosystem II (PSII) embedded in the thylakoid membrane<sup>3</sup>.

Our simulations reveal the dynamics of PSII and its various cofactors on a microsecond time scale. We analyzed the interactions of the thylakoid lipids with PSII and found evidence for the existence of binding sites for specific glycolipids at the membrane-exposed surface of the complex. Furthermore we extensively studied the diffusion of plastoquinone in and out of the PSII, thereby discovering a third plastoquinone/plastoquinol diffusion channel<sup>4</sup>.

1. Marrink, S. J. & Tieleman, D. P. Perspective on the Martini model. *Chem. Soc. Rev.* 42, 6801–6822 (2013).
2. López, C. A., Sovova, Z., van Eerden, F. J., de Vries, A. H. & Marrink, S. J. Martini Force Field Parameters for Glycolipids. *J. Chem. Theory Comput.* 9, 1694–1708 (2013).
3. van Eerden, F. J., de Jong, D. H. & de Vries, A. H. Characterization of thylakoid lipid membranes from cyanobacteria and higher plants by molecular dynamics simulations. *BBA - Biomembranes* (2015).
4. van Eerden, F. J., Melo, M. N., Frederix, P. W. J. M., Periole, X., & Marrink, S. J. (2017). Exchange pathways of plastoquinone and plastoquinol in the photosystem II complex. *Nature Communications*, 8, 15214.



### Date & Time

8<sup>th</sup> Aug. 2017

15:00 - 16:00

### Venue

BIKEN Hall

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