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## Parameterization of Molecular Photoswitches for Martini 3 and their Application in Photopharmacology

*Thursday, 5 March 2026 16:20 (20 minutes)*

Molecular photoswitches are light-responsive compounds that undergo reversible conformational changes upon irradiation. We present Martini 3 coarse-grained models for seven photoswitches, parameterized using semi-empirical reference data and experimental water–octanol partitioning. These models enable the development of digital twins for light-controlled biological systems including membrane modulation, peptide conformational control, and ion channel regulation to study photopharmacology at system sizes and time scales inaccessible to atomistic simulations.

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**Session Classification:** Short Talk