

P034 Coarse grained model of gap junction
trans-membrane domain

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Gap junctions form intercellular channels that mediate metabolic and electrical signaling between neighbouring cells in a tissue. From a molecular point of view the structure of the junction is not known yet. We will present a coarse grained model of the trans membrane domain, based on Monte Carlo simulations and experimental data. The model takes into account only geometrical and steric constraints, and the most important interaction between the aminoacids (i.e. cystein bonds and electromagnetic interactions). These constraints are sufficient to determine geometrical aspects of the gap junction channel, such as the length of the trans-membrane domain, and give some insight on the possible displacements of the extra membrane loops once the gap junction is formed. Possible extensions of the model, towards a full atom modelling of the trans-membrane domain, will be showed.