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Multiscale simulations of neuronal receptors

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Molecular dynamics simulations of proteins may differ by the granularity of the underlying force fields (from quantum to coarse grain). At times, it is very useful to combine different descriptions in a hybrid description. Here I will present recent hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) –and MM/coarse grain (CG) based investigations of targets for pharmaceutical intervention. The predictive power and limitations of these multi-scale methods will be illustrated. The talk will close with a brief survey of multi-scale simulations within the recently formed consortium of the Human Brain Project, one of the two flagships grant funded by the EU.

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