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Investigating membrane proteins by QM/MM MD and machine learning in the Exascale era

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First principle quantum mechanical/molecular mechanics (QM/MM) molecular dynamics (MD) simulations constitute an excellent methodology for the study of quantum phenomena in biological systems. Here we will present QM/MM MD studies from our lab on receptors and transporters. These studies demonstrate the expanding domain of applicability of the approach, thanks to the advent of large parallel machines (such as the exascale computers) and ML.

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