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PhD Thesis: Since 05/2010

Project title: Mathematical characterisation of spatial rearrangements in T-cell receptor – peptide – Major histocompatibility Complex in reaction to agonistic and antagonistic peptides

Project description:

The interaction between T-cell receptor (TCR), peptide (p) and Major Histocompatibility Complex (MHC) is one of the most important processes in the adaptive immune system. A plethora of studies in this context were performed, however the detailed structural trigger is still not known. Therefore, we investigate the spatial rearrangements of TCRpMHC complexes in reaction to agonistic and antagonistic peptides by using splines to characterise the MHC helices, the MHC β -sheets and the complementarity determining regions (CDRs) of the TCR during “in silico” molecular dynamics (MD) simulations.

Hence, this study contributes to the structural understanding of the TCRpMHC interface. We hope to develop a standard method to predict immunogenicity of peptides in interaction with TCR/MHC, based on the overall spatial rearrangement of the TCRpMHC complex.