

In silico approaches:

Docking of gluten peptides to HLA DQ2 and HLA DQ8 as a bioinformatic tool for the prediction of immunotoxic peptides ?

Pierre ROUGÉ



Parma 11.23,2016

docking requirements

templates : HLA DQ2 and HLA DQ8
available at the PDB

HLA DQ2: 1S9V, 4D8P, 4OZF, 4OZI

HLA DQ8: 2NNA, 5KS9, 4Z7U, 4GG6

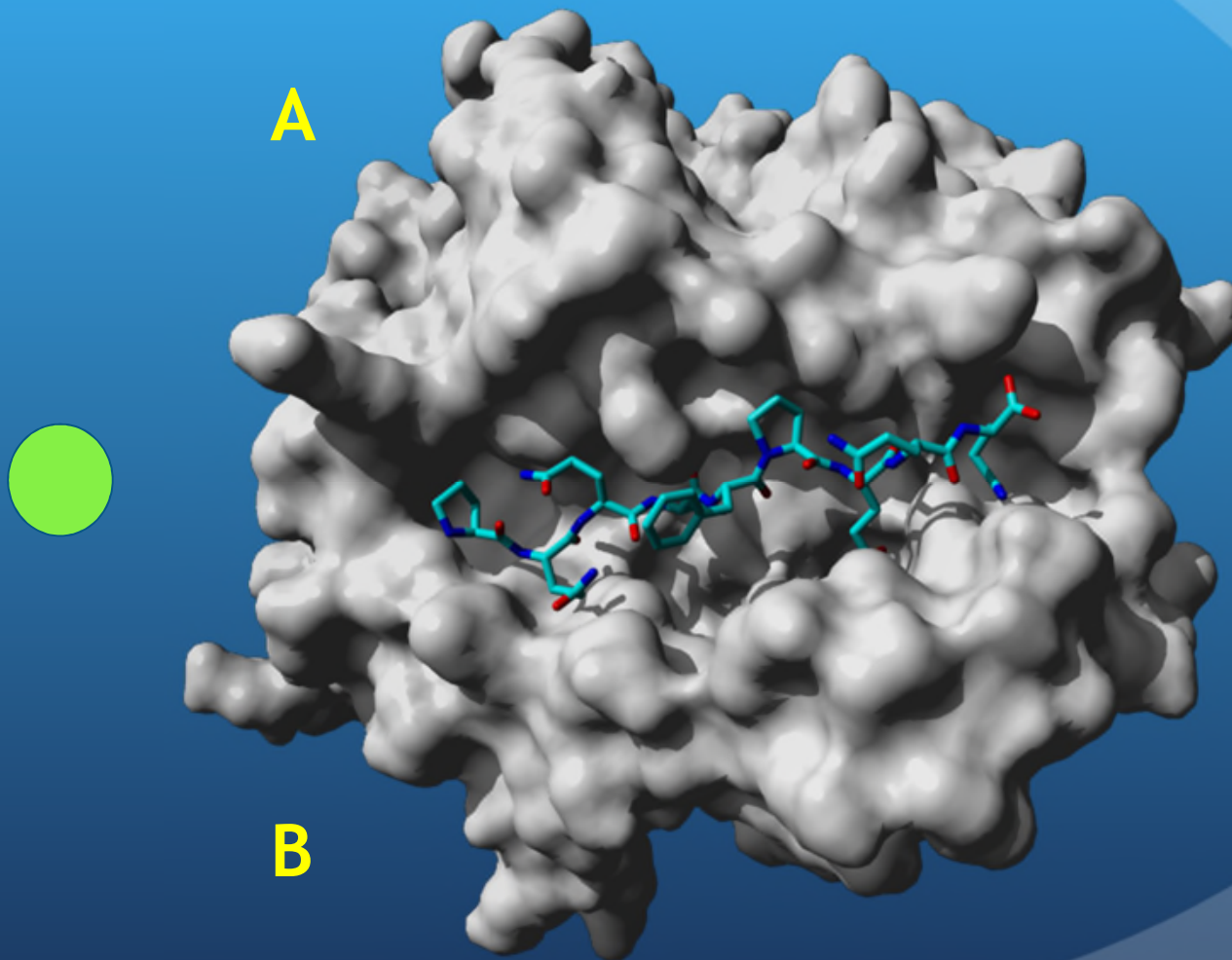
gluten peptides: list of 22 DQ2 and
4 DQ8 peptides

docking/modeling programs

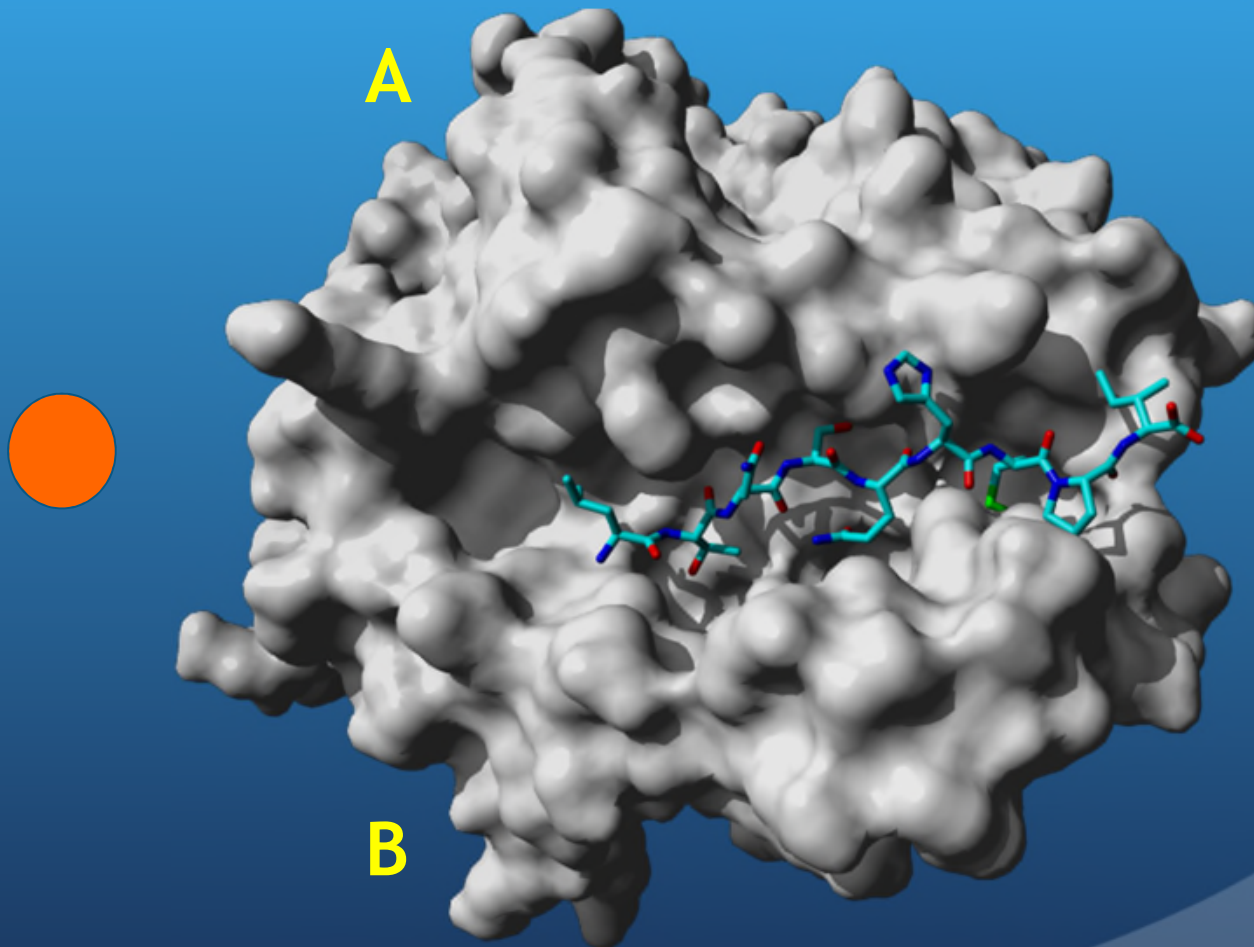
program **GRAMM-X**: available as a web server at grammx@bioinformatics.ku.edu

modeling programs: **Chimera**, **PyMol** and **YASARA** for building the gluten peptides and visualize the docking results

docking results for gluten peptides:
complete fit to the groove = positive result

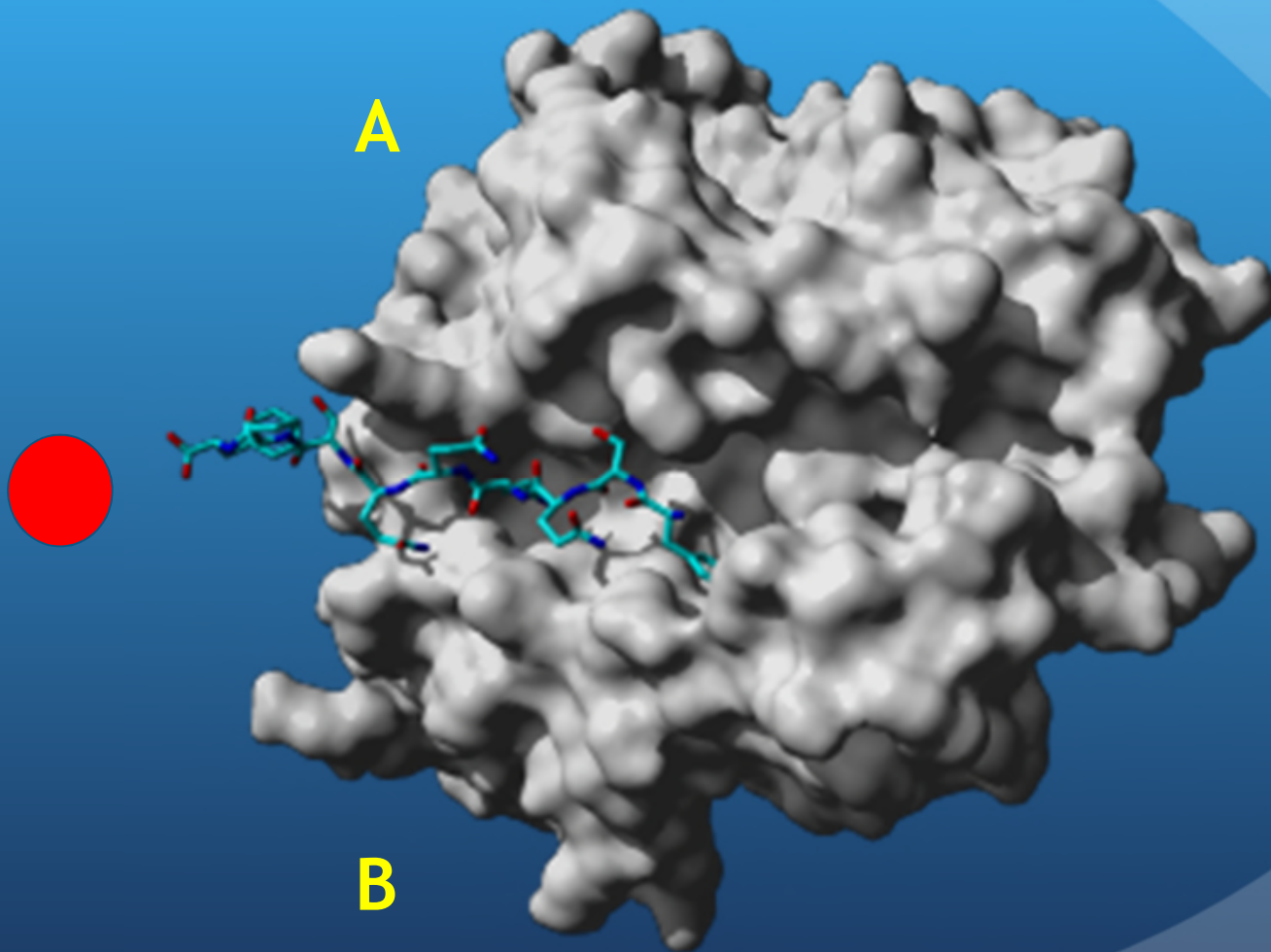


docking results for gluten peptides:
incomplete fit to the groove = negative result



docking results for gluten peptides:

no fit to the groove = negative result

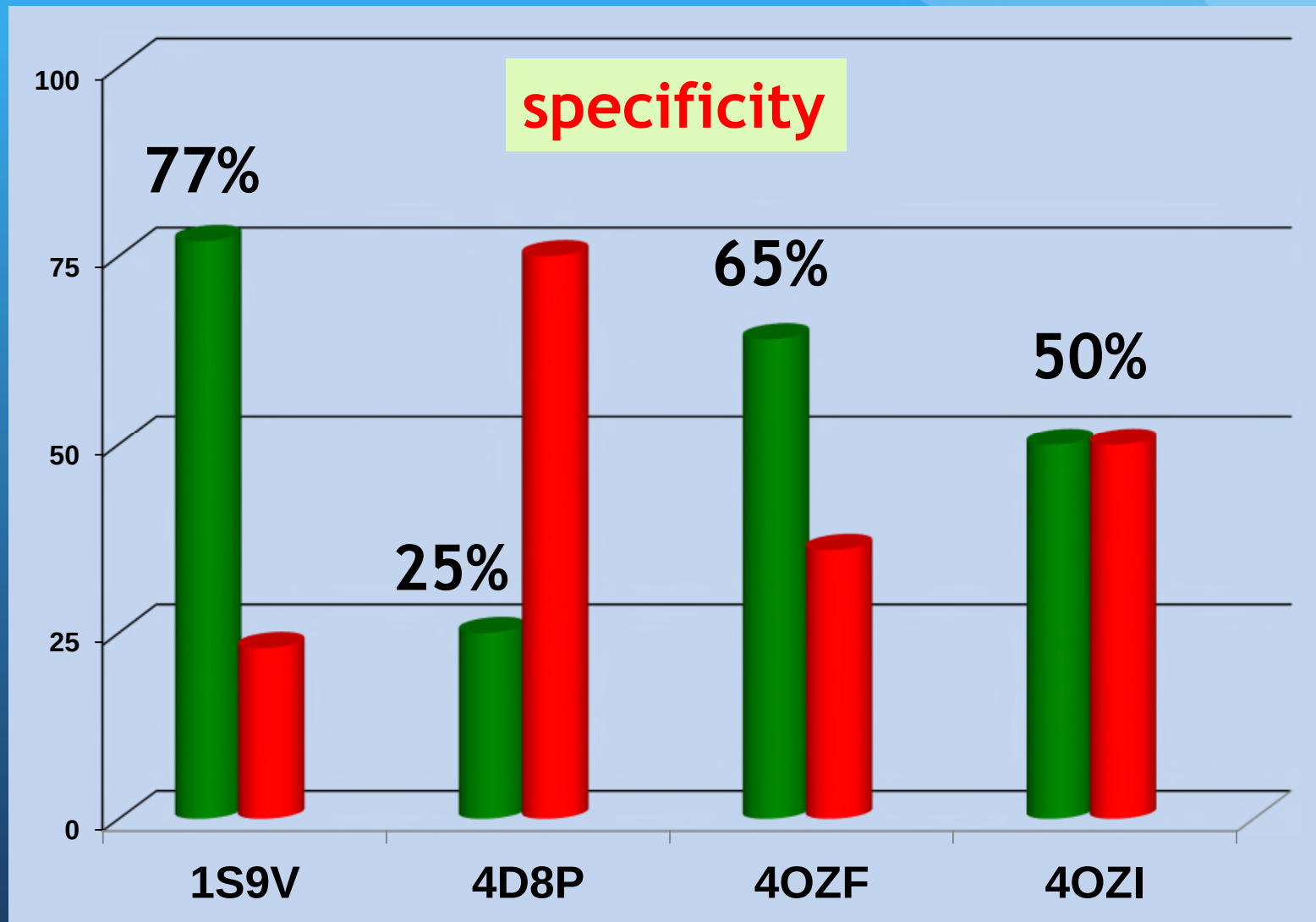


evaluation of docking results

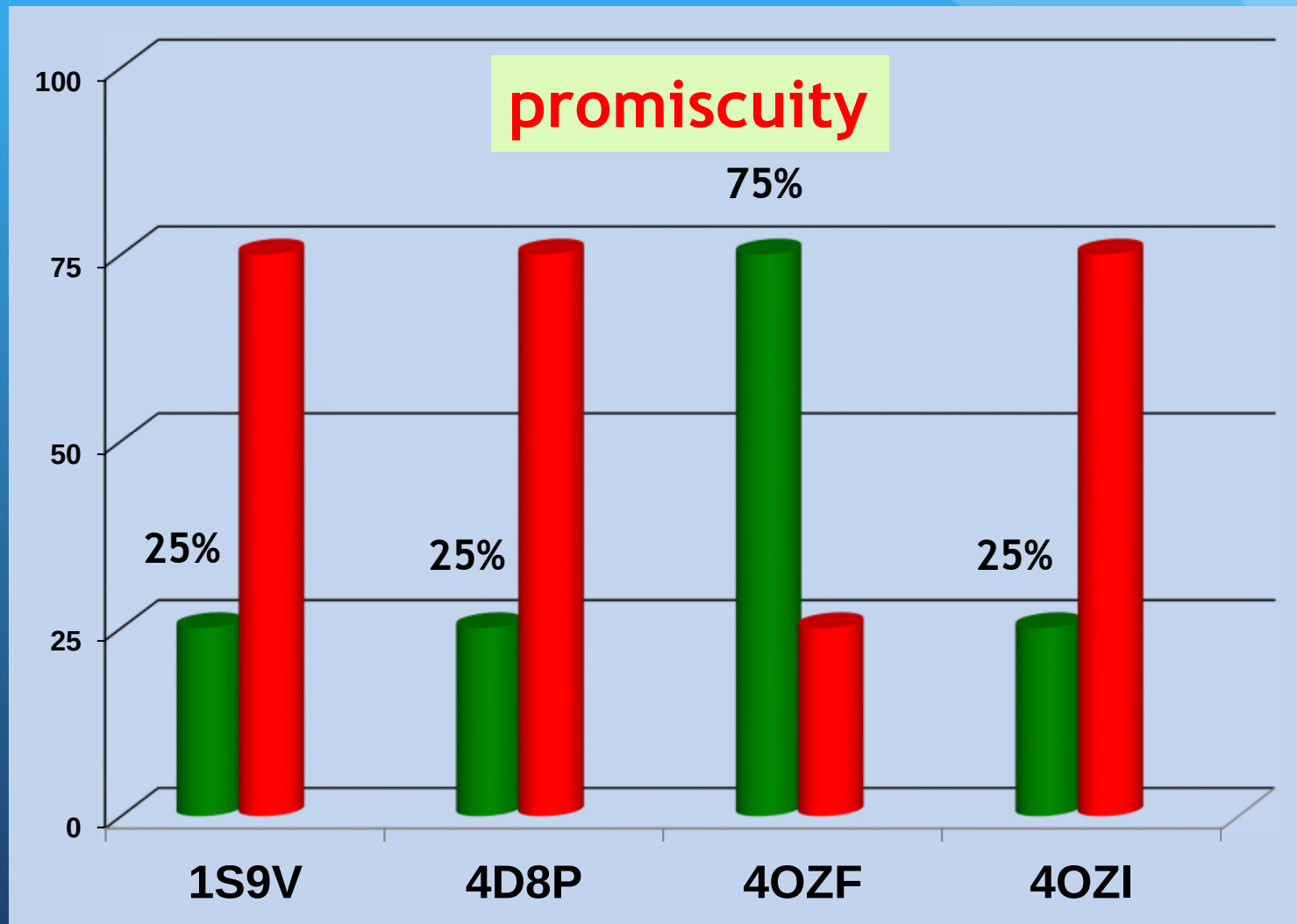
Specificity : percentage of complete fits of DQ2 peptides to HLA DQ2 and DQ8 peptides to HLA DQ8 (homologous interaction)

Promiscuity : percentage of complete fits of DQ8 peptides to HLA DQ2 and DQ2 peptides to HLA DQ8 (heterologous interaction)

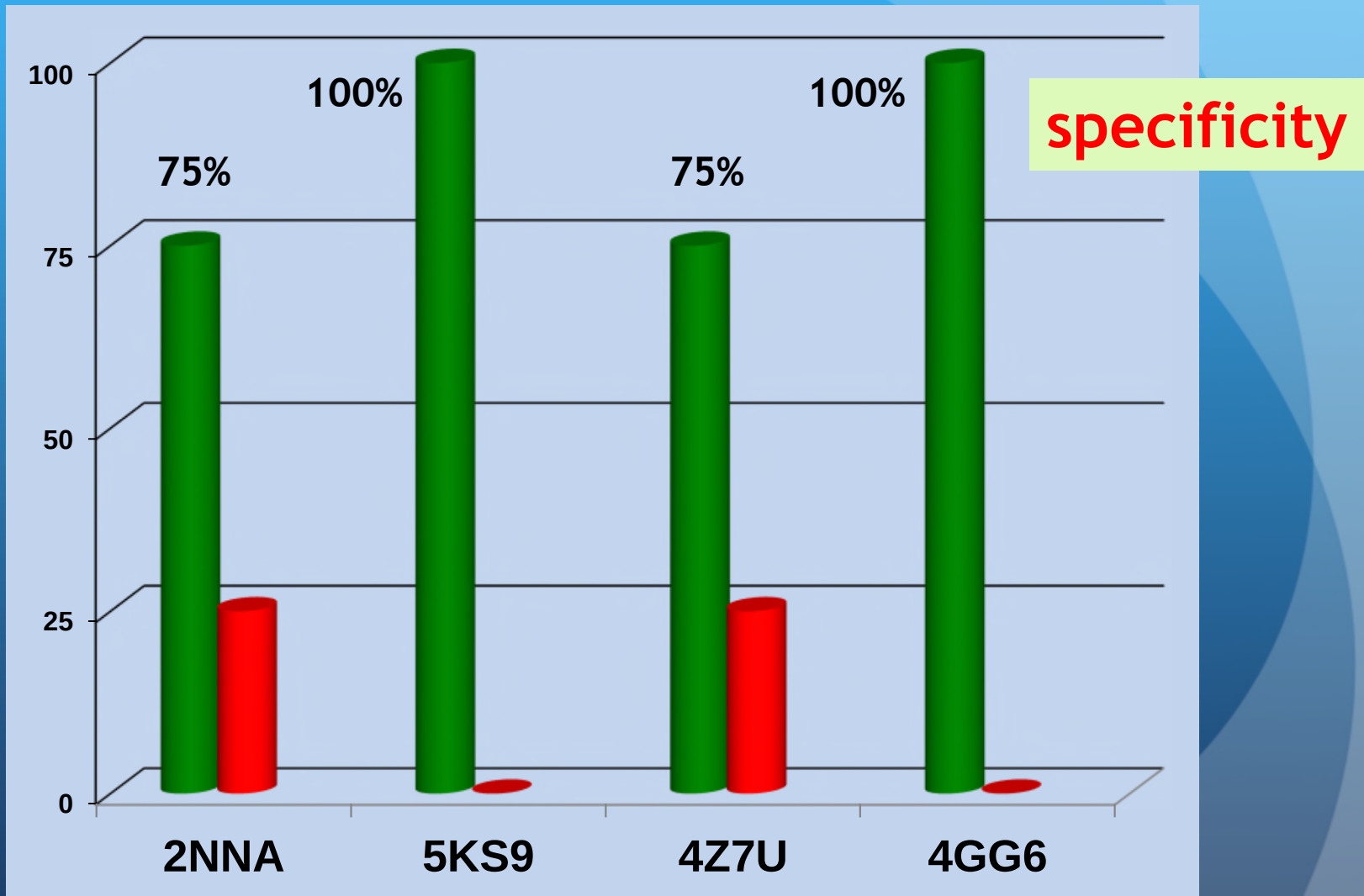
docking of DQ2 peptides to HLA DQ2



docking of DQ8 peptides to HLA DQ2



docking of DQ8 peptides to HLA DQ8



docking of DQ2 peptides to HLA DQ8

