Protein-Protein Docking

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The proteins and/or nucleotides were docked using {HADDOCK 2.4 Webserver|Protein-docking tool} using standard parameters, generating 1000 rigid-body docking decoys, selecting the top 200 structures for semi-flexible and water refinement.

For the generation of active site restraints {random patches|Protein-docking restraints} were defined via the HADDOCK web interface.

For the generation of active site restraints {cross-linking restraints|Protein-docking restraints} were defined as the active site residues.

Contacts between the protein chains were predicted using {Raptor X Complex Contact|Contact prediction tool}.

The peptide was docked using the {ClusPro Webserver|Protein-docking tool}. A six residue length sequence and motif were used as inputs, using the top balanced score to identify the best candidates.