SUPPORTING INFORMATION

Protein-Protein HADDocking using exclusively Pseudocontact Shifts

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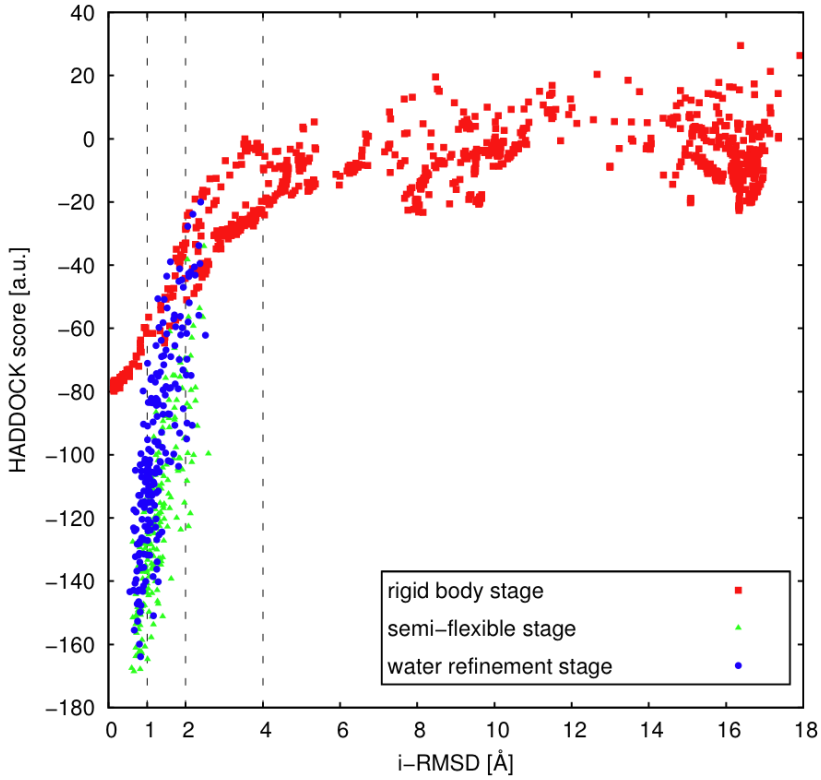
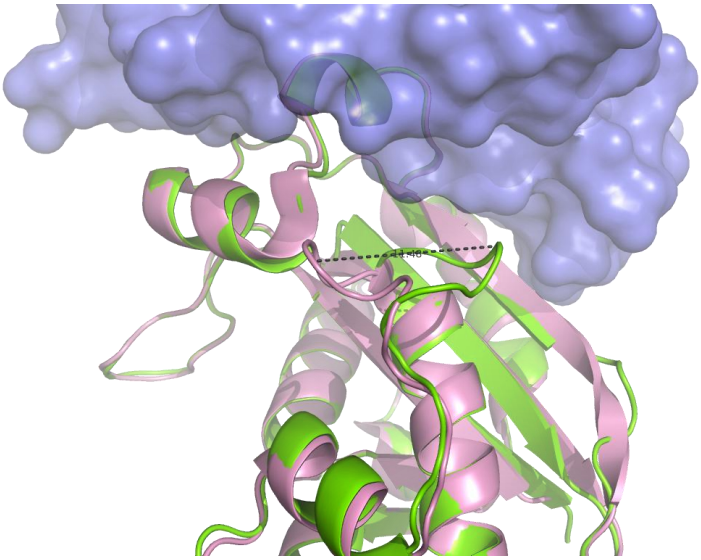
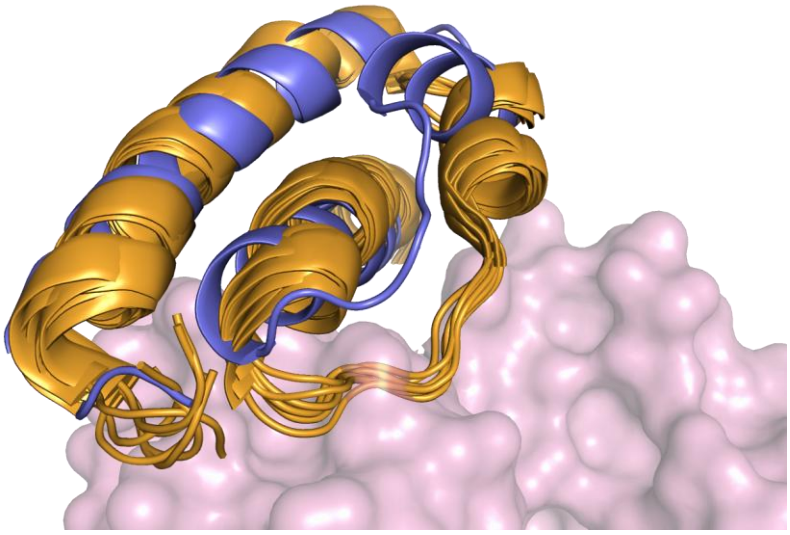


SI Fig. 1 ε186/HOT interface RMSD (i-RMSD) for the intermediate and final results of the bound-bound HADDOCK calculation. The level of noise used for the synthetic data was ± 0.45 ppm. In Figure 1 the level of noise used was ± 0.15 ppm.



SI Fig. 2 Conformational changes of ε186 localized at the loop 157K-162G. In pink the structure of bound ε186 (2IDO chain C). In green the superimposed crystal structure of free ε186 (1J53). In blue the surface of HOT (2IDO chain D). The loop 157K-126G undergoes a large conformational change of up to 11.5 Å.



SI Fig. 3 Conformational changes of HOT. In blue, ribbon representation of bound HOT (2IDO, chain D). In orange, ribbon representation of free HOT (2AXD). In pink, the surface of bound ε186 (2IDO chain C).

SI Table 1 Axial and Rhombic component values used during the docking[a]

	Synthetic PCS[b]			Experimental PCS[c]		
	Dy^{3+}	Er^{3+}	Tb^{3+}	Dy^{3+}	Er^{3+}	Tb^{3+}
$\Delta\chi_{ax}$[d]	10670.0	-2705.4	7282.4	10622.0	-2700.9	7275.0
$\Delta\chi_{rh}$[d]	1252.8	-1130.8	1491.0	1254.9	-1184.9	1554.7

[a] Obtained by fitting the PCS values against ε186 with the software Numbat

[b] The synthetic PCS generated with a level of noise of ± 0.15 ppm are fitted against the bound form of ε186

[c] The experimental PCS are fitted against the unbound form of ε186

[d] In units of $10^{-28}/12/\pi$ m^3