Combining pyDock *ab initio* docking and template-based modeling for the CASP13-CAPRI Challenge

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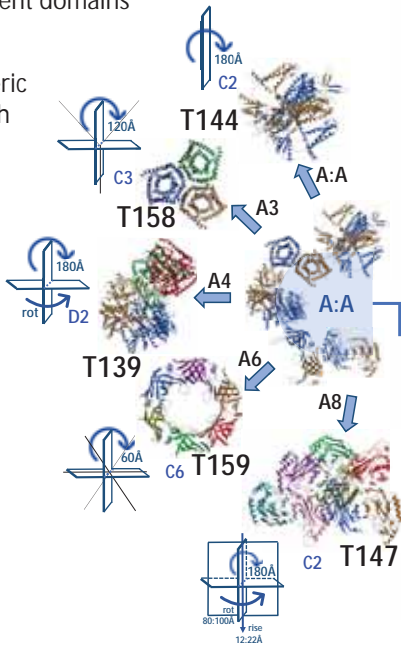*Barcelona Supercomputing Center (BSC), IBMB-CSIC*

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Structural modeling of oligomeric proteins can largely benefit from *ab initio* docking procedures, as part of an integrative approach including template-based data, experimental information on the interface residues, and symmetry restraints.

To evaluate this, we have participated, both as predictors and as scorers, in all the 22 targets proposed for the joint challenge between CASP13 and CAPRI Round 46.
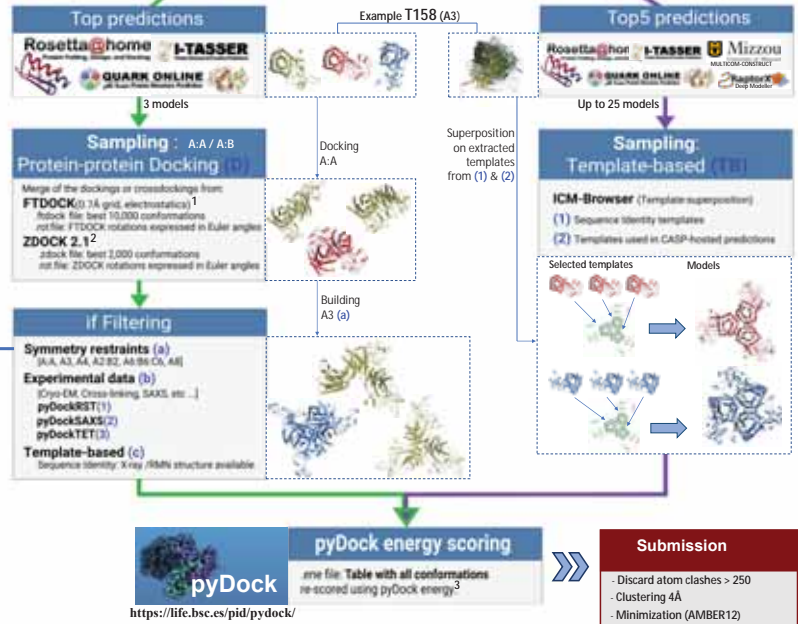
In some targets, the integration of template-based and *ab initio* docking was essential to produce feasible models. In addition, the challenge was not only to model the dimer orientation but also to describe the assembly of the 5 different domains within each monomer.

We scored all models, dimeric and oligomeric models, with pyDock[3], sorting them according to the total binding energy of all possible interfaces.
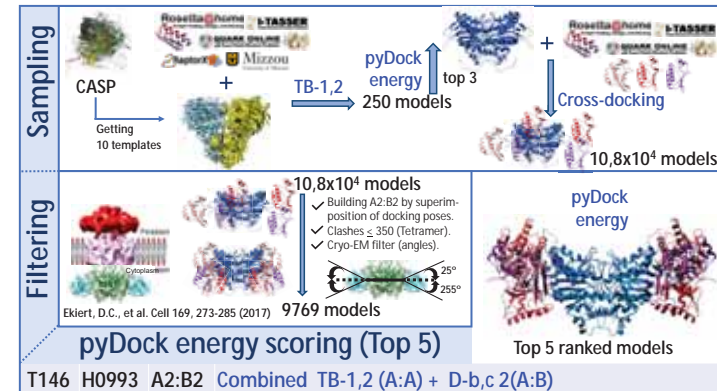
Structural Assembly	CAPRI/CASP target
A:A	T137;T138;T140;T141;T143; T144;T148;T152;T153;T154
A_5D:A_5D	T149-T150-T151
A:B	T142;T155;T156;T157
A3	T158
A2:B2	T146
A4	T139
A8	T147
A6:B6:C6	T159

T146

T146 H0993 A2:B2 Combined TB-1,2 (A:A) + D-b,c 2(A:B)

T159

T159 H1021 A6:B6:C6 Combined TB-1,2 (A)(B)(C) & (B:C) + D-a,c/D-a(A:B:C)

T149-150-151

Sampling
1) FTDOCK standard
2) FTDOCK + pyDockTET[4] + ICM-browser

Filtering
pyDockSAXS[5]
pyDockRST

pyDock energy scoring (Top 5)

T149	T0999	A_5D:A_5D	D-a,b[3] ,c AND D-a
T150	T0999	A_5D:A_5D	D-a,b[2,3],c AND D-a,b[2]
T151	T0999	A_5D:A_5D	D-a,b[1,2,3],c AND D-a,b[1,2]

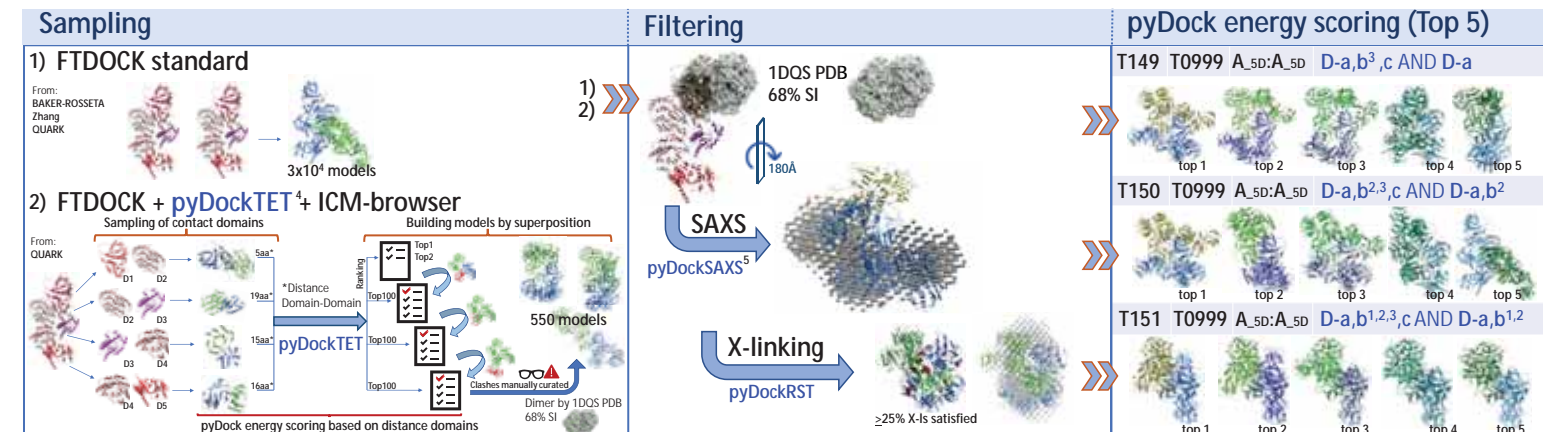**References:**
1. Gabb, H.A., Jackson, R.M. & Sternberg, M.J. Modelling protein docking using shape complementarity, electrostatics and biochemical information. J. Mol. Biol. 272, 106–120 (1997).
2. Chen, R., Li, L. & Weng, Z. ZDOCK: an initial-stage protein-docking algorithm. Proteins 52, 80–87 (2003).
3. Cheng, T.M.-K., Blundell, T.L. & Fernandez-Recio, J. pyDock: electrostatics and desolvation for effective scoring of rigid-body protein-protein docking. Proteins 68, 503–515 (2007).
4. Cheng, T. M.-K., Blundell, T. L. & Fernandez-Recio, J. Structural assembly of two-domain proteins by rigid-body docking. BMC Bioinformatics 9, 441 (2008).
5. Jiménez-García, B., Pons, C., Svergun, D.I., Bernadó, P. & Fernandez-Recio, J. pyDockSAXS: protein-complex structure by SAXS and computational docking. Nucleic Acids Res. 43, W356-361 (2015).