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Type	Oral communication
Session	Structural Bioinformatics
Title	How we Achieved the First Position in the Top-1 and Top-10 Rankings of the CASP13-CAPRI46 Scoring Experiment
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Motivation

Properly scoring protein-protein docking models to single out the correct ones is still an open challenge, also object of assessment in CAPRI (Critical Assessment of PRedicted Interactions), a community-wide blind docking experiment. Traditionally, scoring functions for protein-protein docking poses are energy and/or knowledge based, therefore they calculate a score for each model per se. We introduced in the field CONSRANK (CONSensus RANKing), the first pure consensus method (1). Also available as a web server (2), CONSRANK ranks models based on their ability to match the most conserved (or frequent) inter-residue contacts in the ensemble they belong to. We have been blindly testing CONSRANK in all the latest CAPRI rounds, starting from CAPRI30 (joint experiment with the Critical Assessment of Structure Prediction, CASP11, held during summer 2014), where we showed it to perform competitively with the state-of-the art energy and knowledge based scoring functions (3). More recently, we developed ClustCONSRANK, an algorithm introducing a contact-based clustering of the models as a preliminary step of the CONSRANK scoring process (4).
In the latest CASP13-CAPRI46 joint experiment, held between May and August 2018, we participated as scorers with a novel pipeline, combining both our scoring tools, CONSRANK and ClustCONSRANK, with our interface analysis tool COCOMAPS (5). Results of such an approach are presented here.

Methods

For scoring all the CASP13-CAPRI46 targets (with the exception of T159, see below), we relied on our scoring tools CONSRANK and ClustCONSRANK. Models top ranked by CONSRANK and ClustCONSRANK were further analyzed with COCOMAPS, a web tool we developed for the analysis of the interface in macromolecular biocomplexes. Selection of the 10 models for submission was guided by the strength of the emerging consensus, and their final ranking was assisted by results of the interface analysis. The above approach was entirely based on methods made available to the community as web tools, and could thus be reproduced by any user. As CONSRANK could not be applied to the 18-mer target T159, a completely different approach, based on short molecular dynamics simulations in vacuo, was used for it.

Results

Results of the assessment of the CASP13-CAPRI46 scoring experiment are reported in the Figure. Based on the comparison between predictions and the final experimental structures of the target complexes, CAPRI assessors classify correct models, in order of increasing quality, as acceptable, medium or high quality.
We submitted scoring predictions for all the 19 assessed targets. As a result of the above described approach, we were by far the first scorer in the top-1 ranking, having medium/high quality models ranked at the top-1 position for the majority of targets (11 out of the total 19, see Figure). Which compares with the 7 high/medium quality, plus 1 acceptable model, of the second scorer in this ranking.
We were also the best performing scorer group in the top-10 ranking (see Figure), on a par with the Fernandez-Recio’s group, with 11 targets having high/medium quality models, plus 1 target having acceptable models. In the top-5 ranking, we were second after Fernandez-Recio having the same number of targets with correct solutions, 12, but 1 target less with high quality models, 4 vs. 5.
Introducing some flexibility in the final model selection and ranking, as well as differentiating the adopted scoring approach depending on the targets were probably the key assets for our highly successful performance, as compared to previous CAPRI rounds. Details on the adopted protocol and results for individual targets will be given and discussed in the presentation.

Info

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Figure

Assessment results of the CASP13-CAPRI46 scoring experiment

Scorer Group	Rank	Top-1	Rank	Top-5	Rank	Top-10
Fernandez-Recio	3	7/2***/5**	1	12/5***/6**	1	12/5***/6**
Oliva	1	11/4***/7**	2	12/4***/7**	1	12/5***/6**
Kihara	6	9/1***/7**	3	11/3***/6**	3	12/5***/5**
Huang	2	8/2***/5**	4	11/3***/6**	5	12/4***/6**
LZERD	12	10/8**	5	10/3***/6**	4	11/5***/4**
Carbone	7	8/1***/7**	6	9/3***/5**	11	11/3***/6**
Zou	12	10/8**	7	12/2***/9**	6	13/3***/8**
Chang	4	10/1***/8**	8	11/2***/9**	8	12/3***/8**
MDOCKPEP	8	8/1***/6**	9	13/2***/8**	6	13/3***/8**
Venclovas	4	10/1***/8**	10	11/2***/8**	12	13/2***/10**
Bates	14	8/6**	11	11/2***/7**	13	11/2***/8**
HAWKDOCK	9	4/1***/3**	12	5/2***/3**	16	6/2***/4**
HDOCK	11	9**	13	12/1***/10**	8	12/3***/8**
Bonvin	15	8/5**	14	12/1***/7**	10	12/3***/6**
Weng	16	6/5**	15	9/1***/6**	17	12/1***/9**
Seok	9	4/1***/3**	16	8/1***/5**	14	10/2***/5**
Grudinin	17	5**	17	6/1***/5**	15	8/2***/5**
QASDOM	18	3**	18	5**	18	7**

For each ranking (Top-1/5/10), the number of targets for which at least one correct/high***/medium** quality model was submitted is reported

Top-1: only the 1st top ranked model per target is considered
Top-5: only the 5 top ranked models per target are considered
Top-10: all the 10 submitted models per target are considered

Availability	https://www.molnac.unisa.it/BioTools/consrank/

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