APOLLO: a quality assessment service for single and multiple protein models
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ABSTRACT
Summary: We built a web server named APOLLO, which can evaluate the absolute global and local qualities of a single protein model using machine learning methods or the global and local qualities of a pool of models using a pair-wise comparison approach. Based on our evaluations on 107 CASP9 (Critical Assessment of Techniques for Protein Structure Prediction) targets, the predicted quality scores generated from our machine learning and pair-wise methods have an average per-target correlation of 0.671 and 0.917, respectively, with the true model quality scores. Based on our test on 92 CASP9 targets, our predicted absolute local qualities have an average difference of 2.60 Å with the actual distances to native structure.

Availability: http://sysbio.rnet.missouri.edu/apollo/. Single and pair-wise global quality assessment software is also available at the site.

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1 INTRODUCTION

Protein model quality assessment plays an important role in protein structure prediction and application. Assessing the quality of protein models is essential for ranking models, refining models and using models (Cheng, 2008). Model Quality Assessment Programs (MQAPs) predict model qualities from two perspectives: the global quality of the entire model and the residue-specific local qualities. The techniques often used by MQAPs include multiple-model (clustering) methods (Ginalski et al., 2003; McGuirf, 2007, 2008; Paluszewski and Karpus, 2008; Wallner and Elofsson, 2007; Zhang and Skolnick, 2004a), single model methods (Archie and Karpus, 2009; Benkert et al., 2008; Cline et al., 2002; Qiu et al., 2008; Wallner and Elofsson, 2003; Wang et al., 2008) and hybrid methods (Cheng et al., 2009; McGuirf, 2009).

According to the CASP experiments, multiple-model clustering methods are currently more accurate than single model methods. However, they cannot work well if only a small number of models are available. A hybrid quality assessment method (Cheng et al., 2009) was recently developed to combine the two approaches and integrate their respective strengths. Here, we build a web server to provide the community with access to all three model quality assessment approaches (i.e. single, clustering and hybrid).
These PDB files were preprocessed in order to select correct chains to the average of all the models is computed as:

correlation of our pair-wise local quality predictions is 0.053, which is also among the top local quality predictors in CASP9. We also conducted a blind test of the absolute local quality predictor (trained on the CASP8 dataset) on the CASP9 models of 92 CASP9 single domain proteins. On the residues whose actual distances to the native are ≤ 10 and 20 Å, the average absolute difference between our predicted distances and the actual distances is 2.60 and 3.18 Å, respectively.

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**Conflict of Interest:** none declared.

**REFERENCES**


**Table 1. Results of global quality assessment methods used by APOLLO server on 107 CASP9 targets**

<table>
<thead>
<tr>
<th>Methods</th>
<th>Average correlation</th>
<th>Average top 1</th>
<th>Overall correlation</th>
<th>Average loss</th>
</tr>
</thead>
<tbody>
<tr>
<td>Absolute score</td>
<td>0.671</td>
<td>0.552</td>
<td>0.767</td>
<td>0.095</td>
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<tr>
<td>Average pair-wise GDT-TS</td>
<td>0.917</td>
<td>0.591</td>
<td>0.943</td>
<td>0.057</td>
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<tr>
<td>Refined absolute score</td>
<td>0.870</td>
<td>0.567</td>
<td>0.928</td>
<td>0.081</td>
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<tr>
<td>Refined pair-wise Q-score</td>
<td>0.835</td>
<td>0.572</td>
<td>0.904</td>
<td>0.076</td>
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</tbody>
</table>