Assessment of ligand-binding residue predictions in CASP9

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Interactions between proteins and their ligands play central roles in many physiological processes. The structural details for most of these interactions, however, have not yet been characterized experientially. Therefore, various computational tools have been developed to predict the location of binding sites and the amino acid residues interacting with ligands. In this manuscript, we assess the performance of 33 methods participating in the ligand-binding site prediction category in CASP9. The overall accuracy of ligand-binding site predictions in CASP9 appears rather high (average Matthews correlation coefficient of 0.62 for the 10 top performing groups) and compared to previous experiments more groups performed equally well. However, this should be seen in context of a strong bias in the test data toward easy template-based models. Overall, the top performing methods have converged to a similar approach using ligand-binding site inference from related homologous structures, which limits their applicability for difficult de novo prediction targets. Here, we present the results of the CASP9 assessment of the ligand-binding site category, discuss examples for successful and challenging prediction targets in CASP9, and finally suggest changes in the format of the experiment to overcome the current limitations of the assessment. Proteins 2011. ‖ 2011 Wiley-Liss, Inc.

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