Supplementary figures for "Consistent probabilistic outputs for protein function prediction"

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Contents

1 Per term evaluation

1.1 Bar plots by ontology

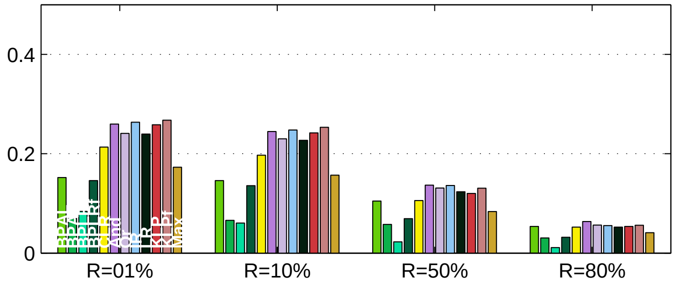

Figure S.1: **Proteins retrieved for a fixed GO term for the Biological Process ontology (hold-out set)** In average over GO terms with the same recall levels: precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$.

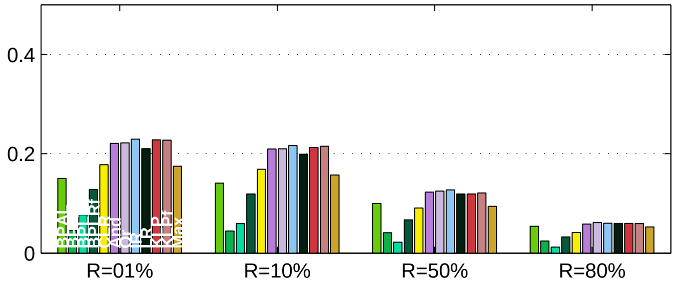

Figure S.2: **Proteins retrieved for a fixed GO term for the Biological Process ontology (test set)** In average over GO terms with the same recall levels: precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$.

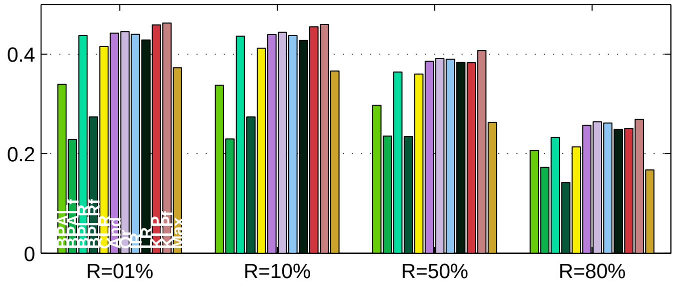

Figure S.3: **Proteins retrieved for a fixed GO term for the Molecular Function ontology (hold-out set)** In average over GO terms with the same recall levels: precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$.

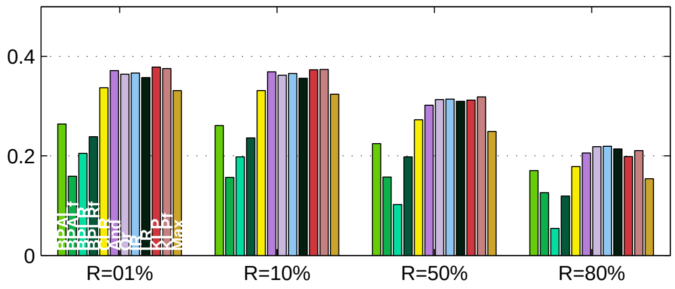

Figure S.4: **Proteins retrieved for a fixed GO term for the Molecular Function ontology (test set)** In average over GO terms with the same recall levels: precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$.

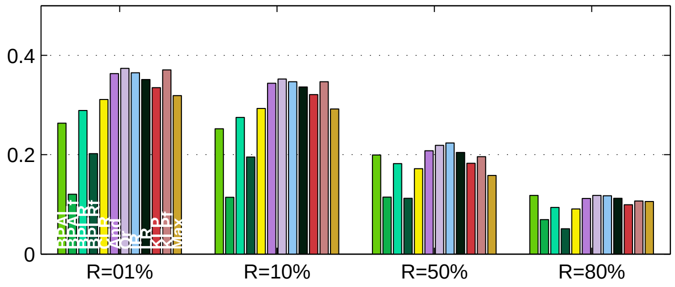

Figure S.5: **Proteins retrieved for a fixed GO term for the Cellular Component ontology (hold-out set)** In average over GO terms with the same recall levels: precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$.

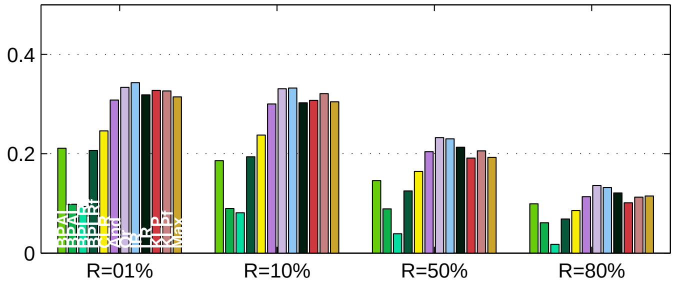

Figure S.6: **Proteins retrieved for a fixed GO term for the Cellular Component ontology (test set)** In average over GO terms with the same recall levels: precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$.

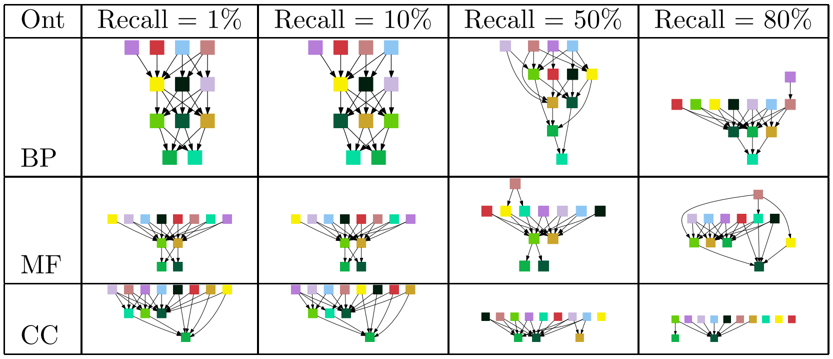

Figure S.7: **Statistical significance testing of per term evaluation, irrespective of term size.** Each panel shows a directed graph in which nodes are methods and a directed edge from node *A* to node *B* indicates that method *A* performs significantly better than method *B* according to the Z-test.

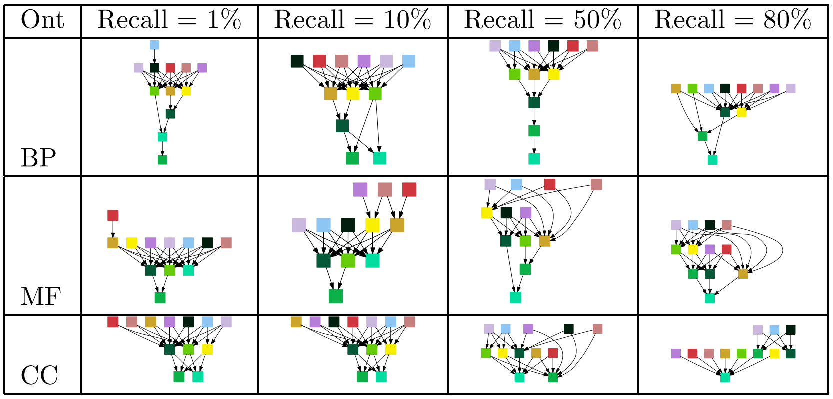

Figure S.8: **Statistical significance testing of per term evaluation, irrespective of term size.** Each panel shows a directed graph in which nodes are methods and a directed edge from node *A* to node *B* indicates that method *A* performs significantly better than method *B* according to the Z-test.

1.2 Directed graphs by ontology

1.3 Bar plots by ontology and term size

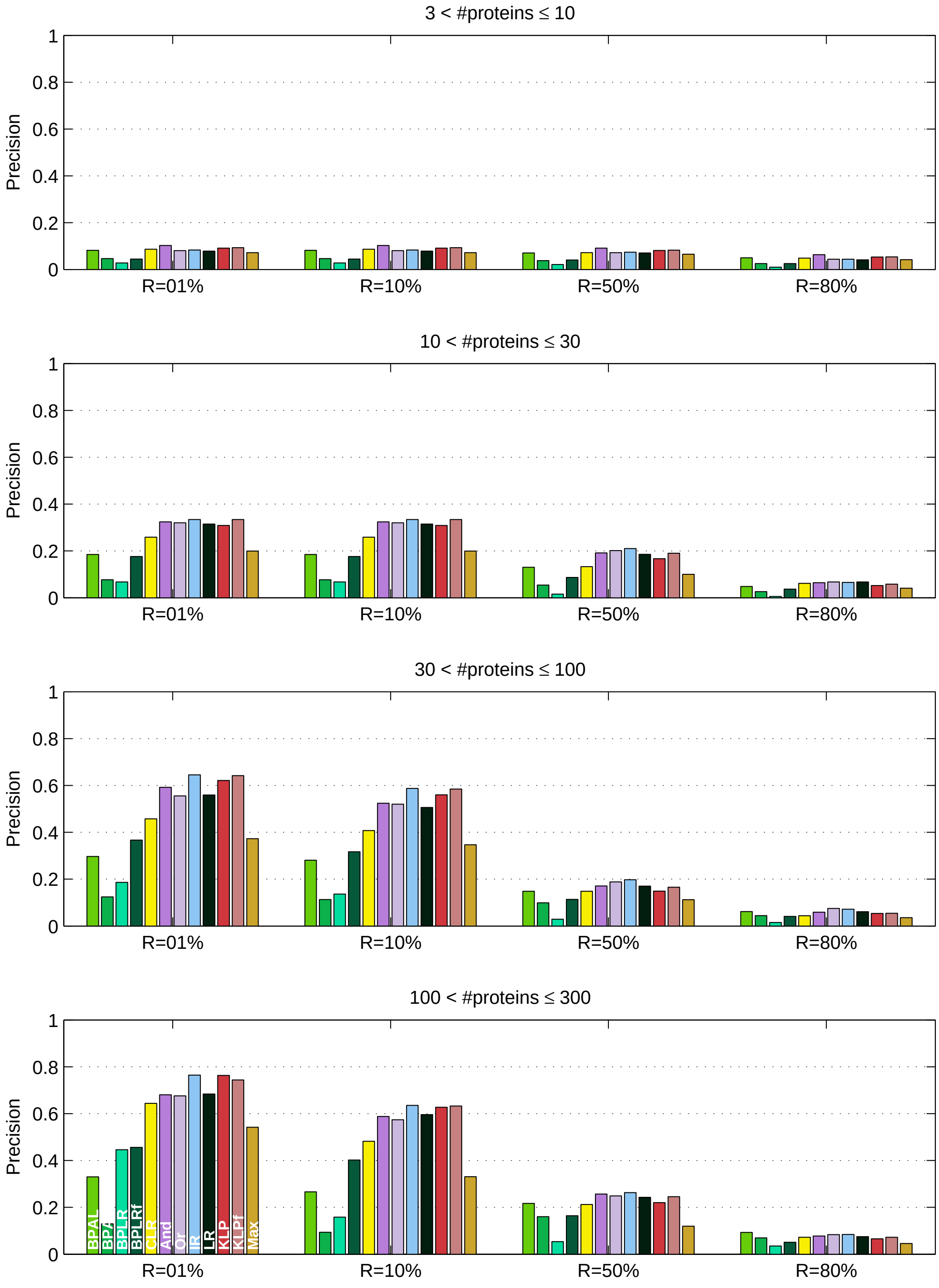

Figure S.9: **Proteins retrieved for a fixed GO term for the Biological Process ontology (hold-out set)** In average over GO terms with the same recall levels: precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$. GO terms are grouped by size.

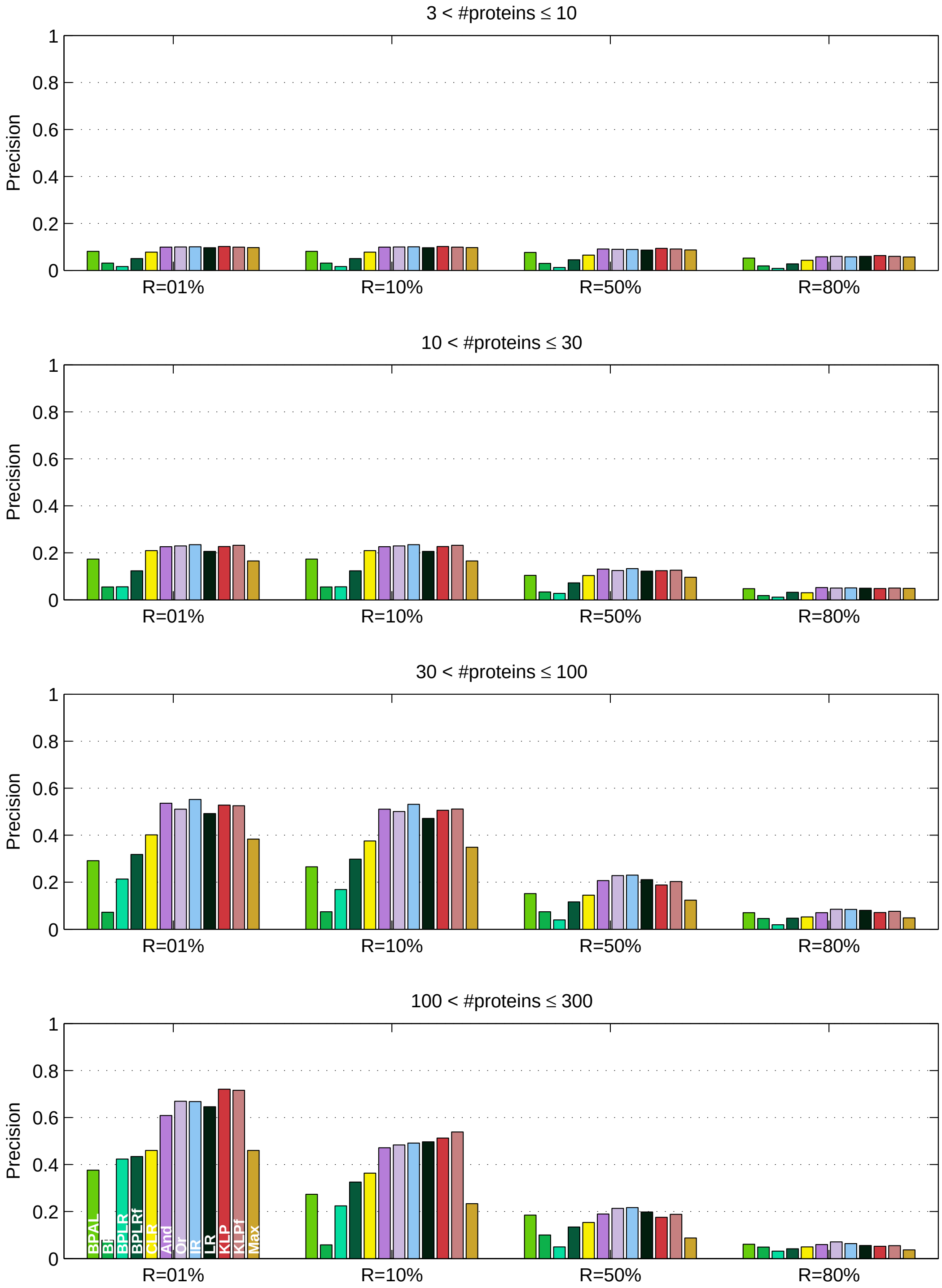

Figure S.10: **Proteins retrieved for a fixed GO term for the Biological Process ontology (test set)** In average over GO terms with the same recall levels: precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$. GO terms are grouped by size.

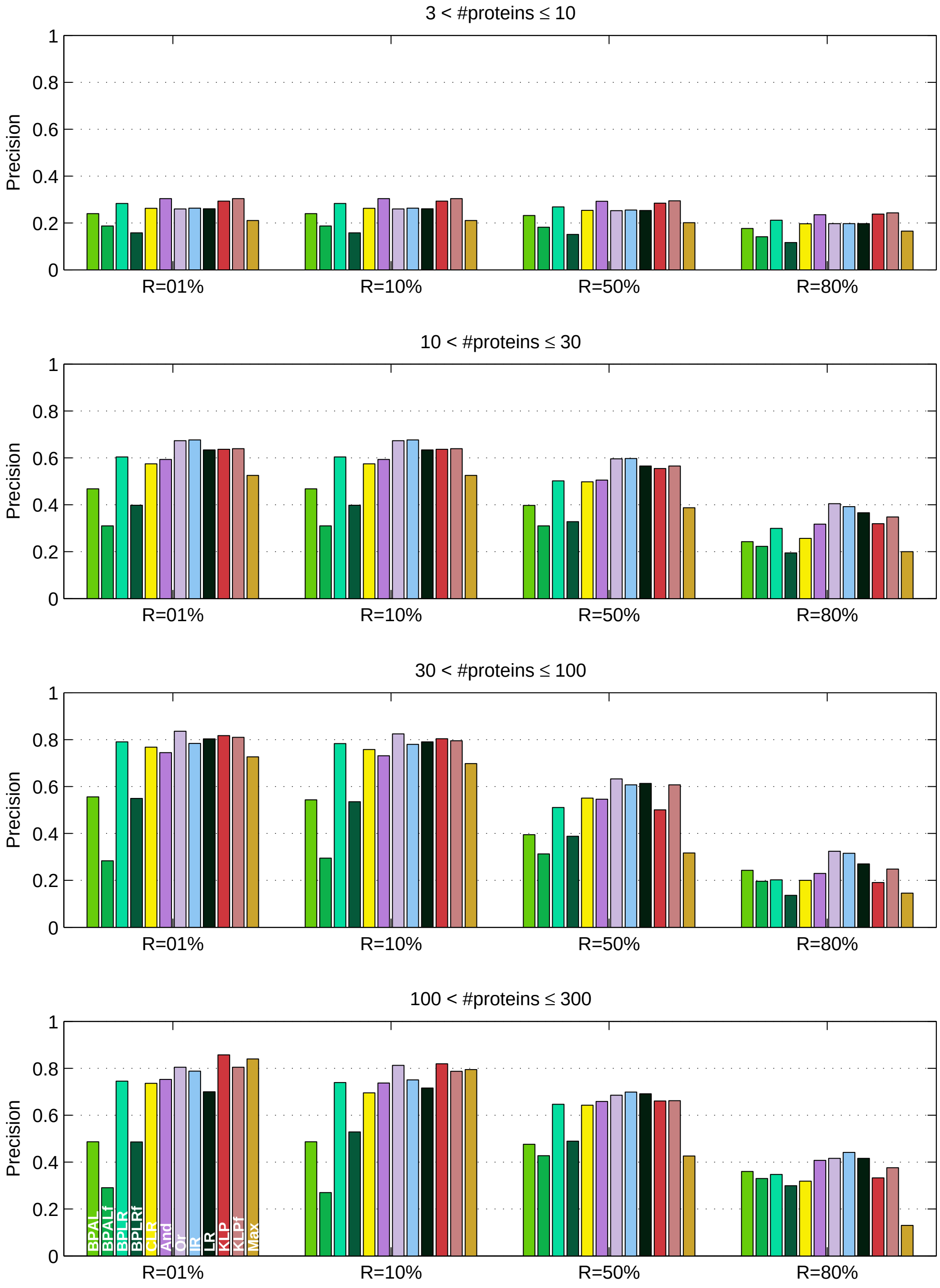

Figure S.11: **Proteins retrieved for a fixed GO term for the Molecular Function ontology (hold-out set)** In average over GO terms with the same recall levels: precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$. GO terms are grouped by size.

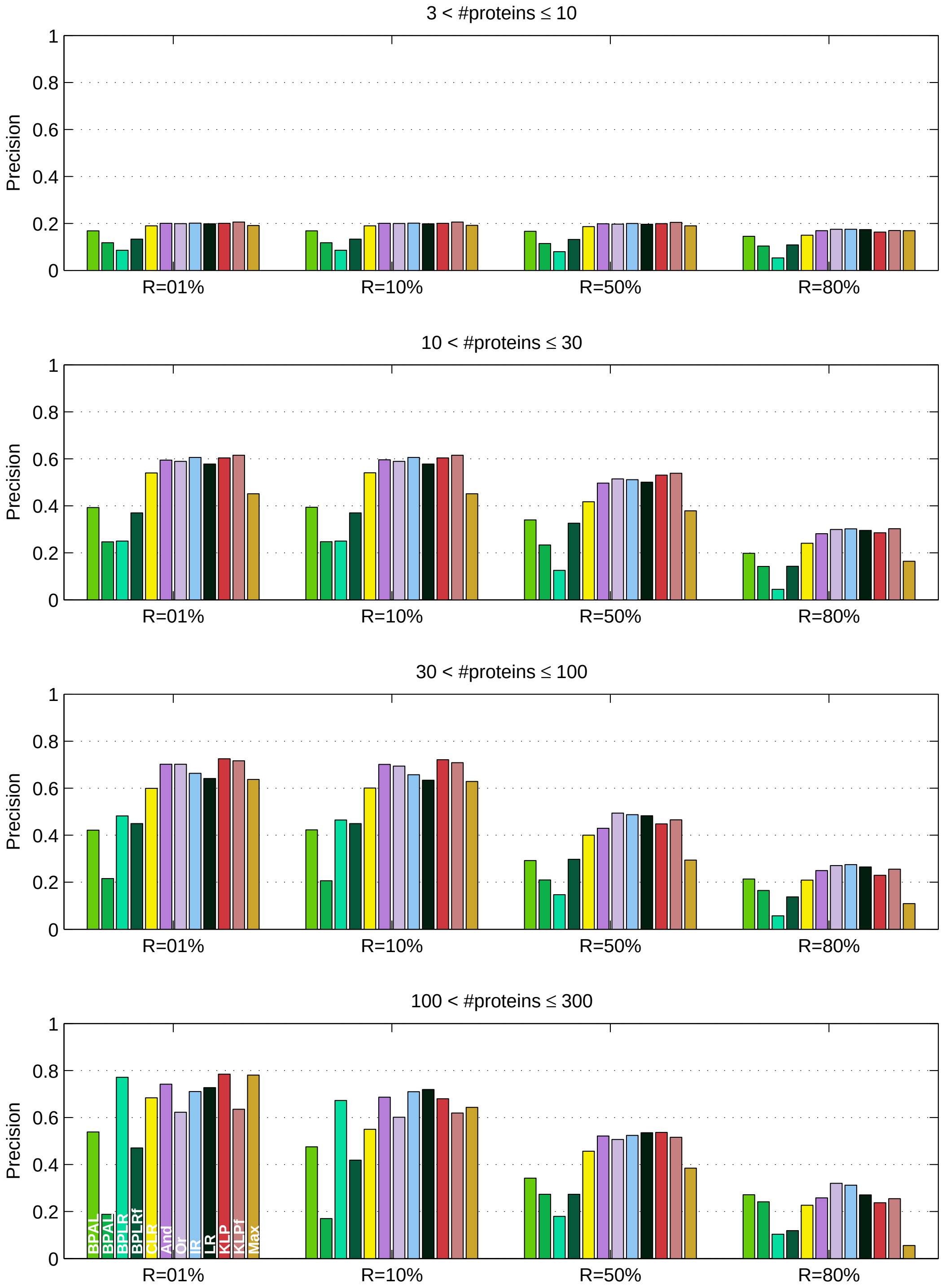

Figure S.12: **Proteins retrieved for a fixed GO term for the Molecular Function ontology (test set)** In average over GO terms with the same recall levels: precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$. GO terms are grouped by size.

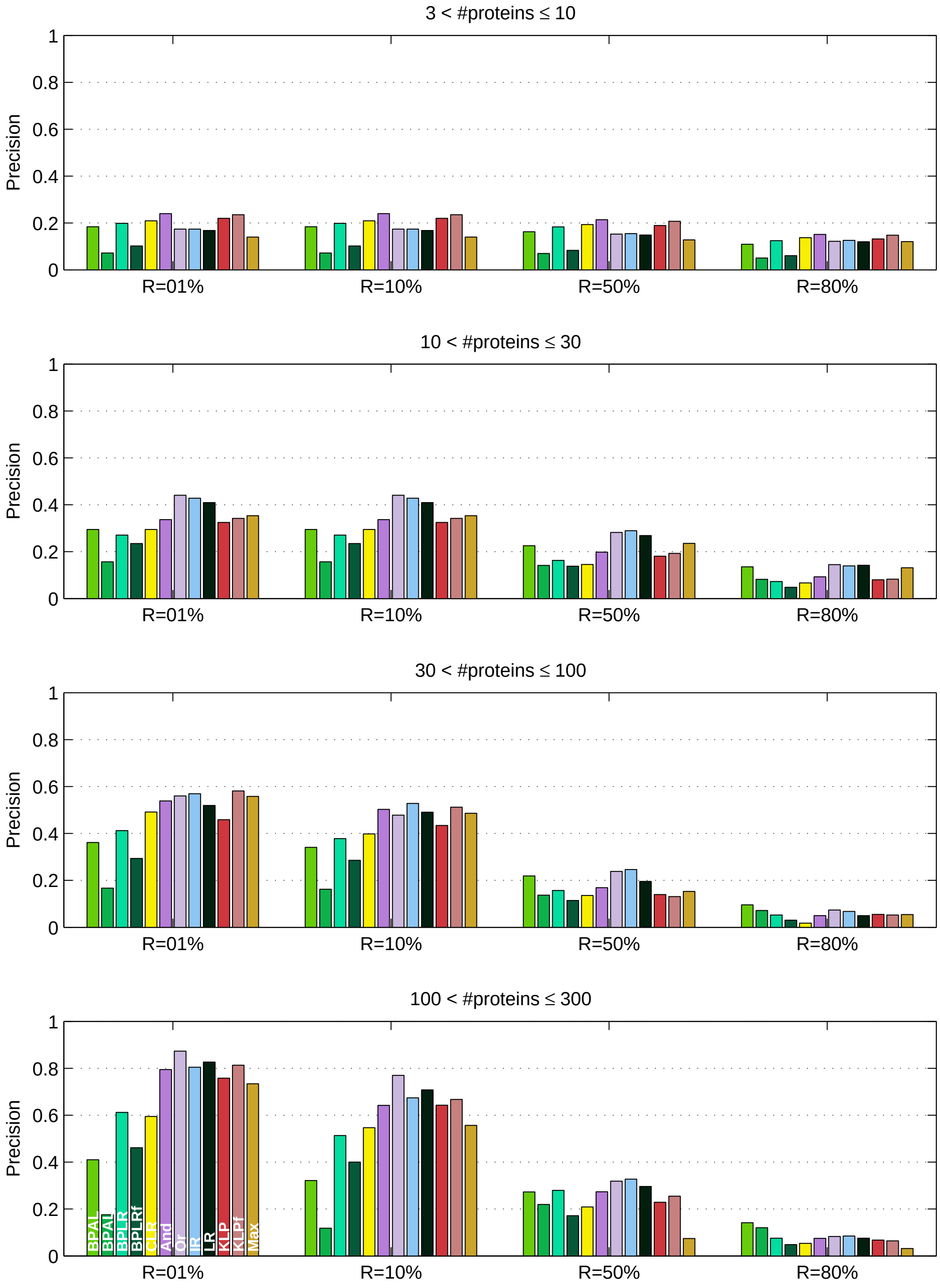

Figure S.13: **Proteins retrieved for a fixed GO term for the Cellular Component ontology (hold-out set)** In average over GO terms with the same recall levels: precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$. GO terms are grouped by size.

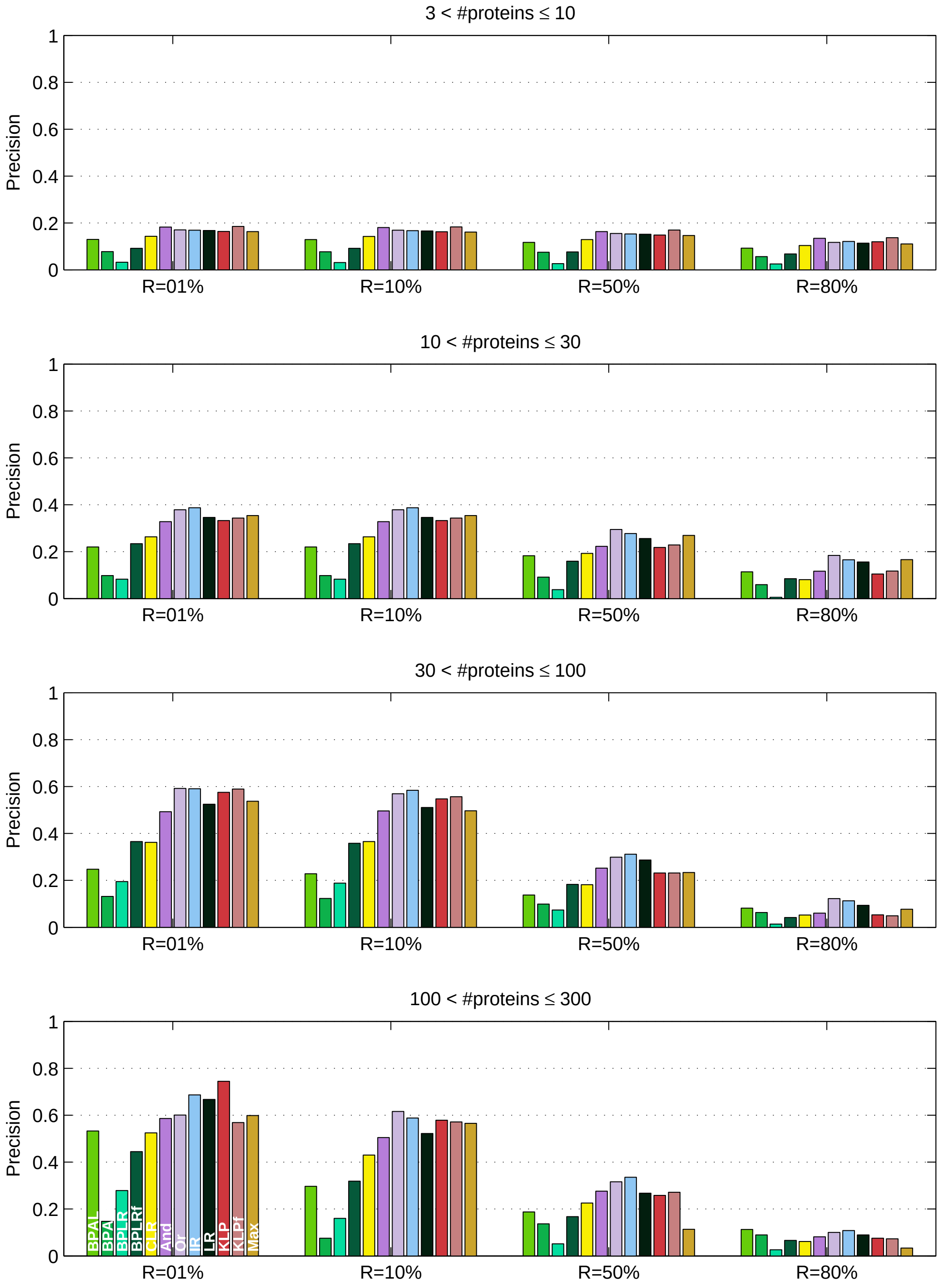

Figure S.14: **Proteins retrieved for a fixed GO term for the Cellular Component ontology (test set)** In average over GO terms with the same recall levels: precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$. GO terms are grouped by size.

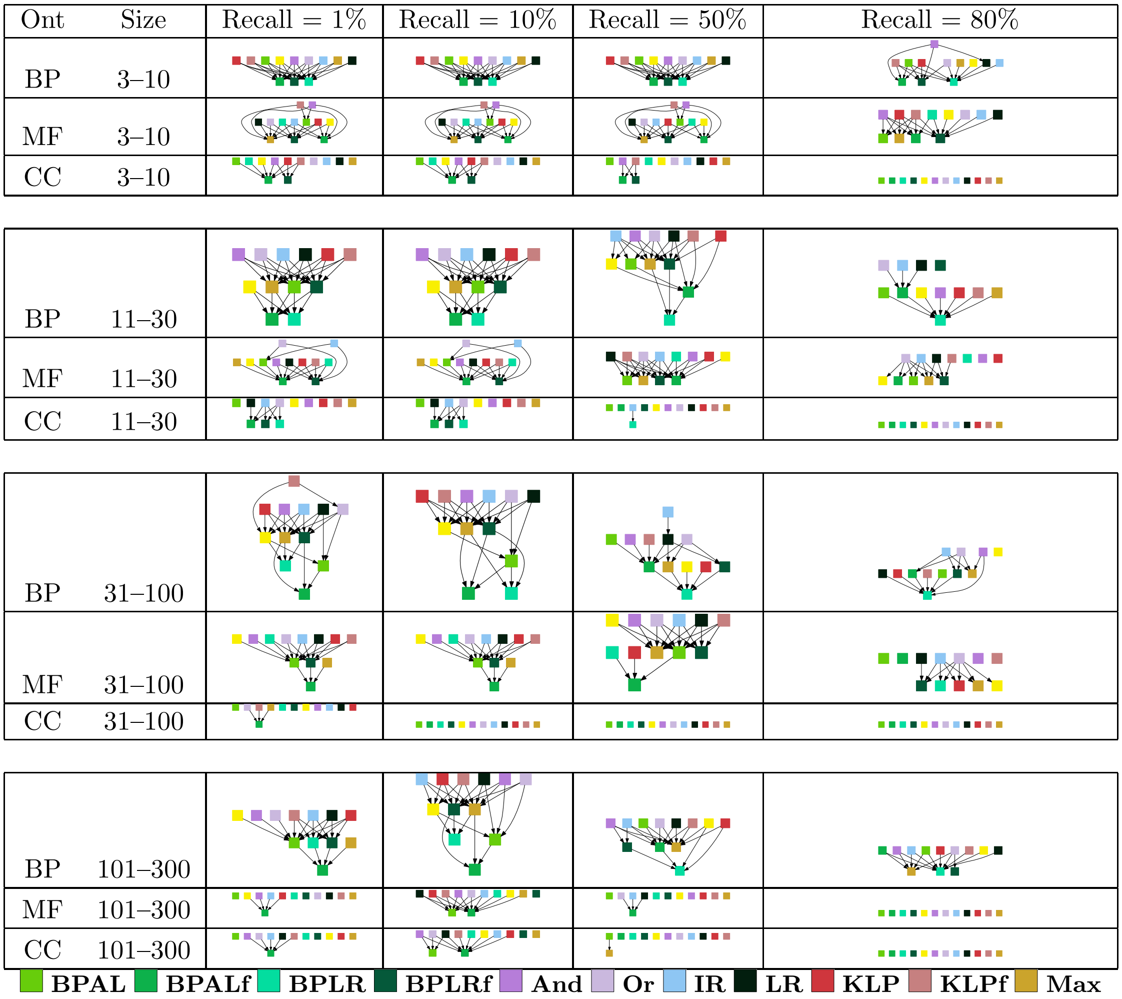

Figure S.15: **Statistical significance testing of per term evaluation** Each panel shows a directed graph in which nodes are methods and a directed edge from node A to node B indicates that method A performs significantly better than method B according to the Z-test.

1.4 Directed graphs by ontology and term size

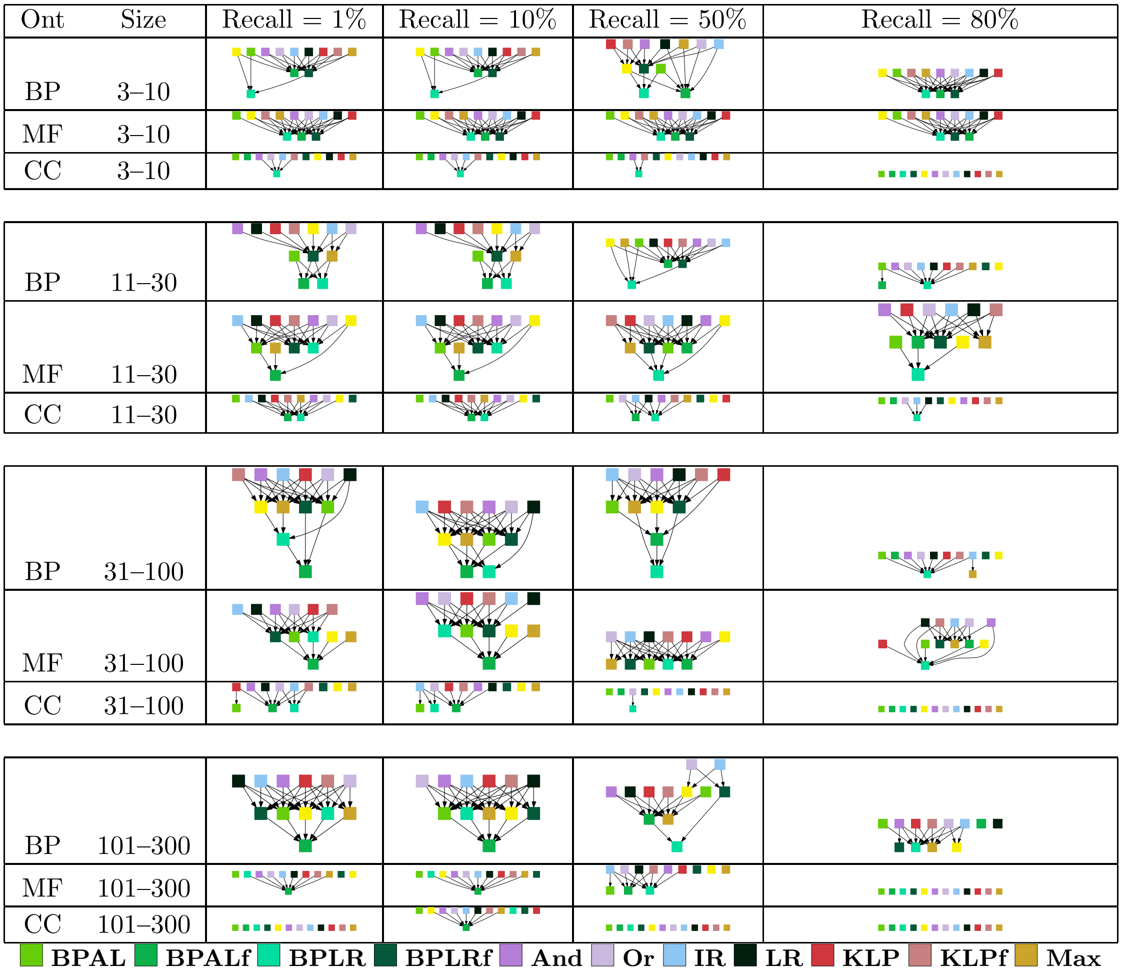

Figure S.16: **Statistical significance testing of per term evaluation** Each panel shows a directed graph in which nodes are methods and a directed edge from node A to node B indicates that method A performs significantly better than method B according to the Z-test.

2 Per protein evaluation

2.1 Bar plots by ontology

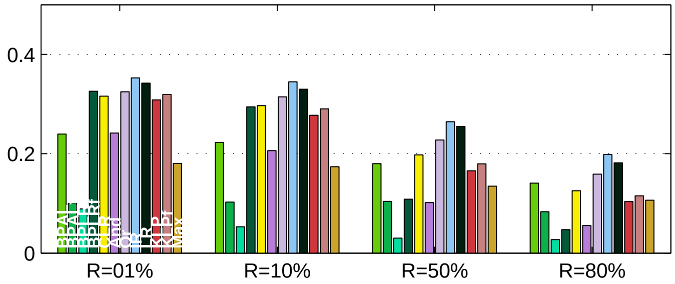

Figure S.17: **GO terms correctly found for a given protein for the Biological Process ontology (hold-out set)** Average over proteins of the precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$.

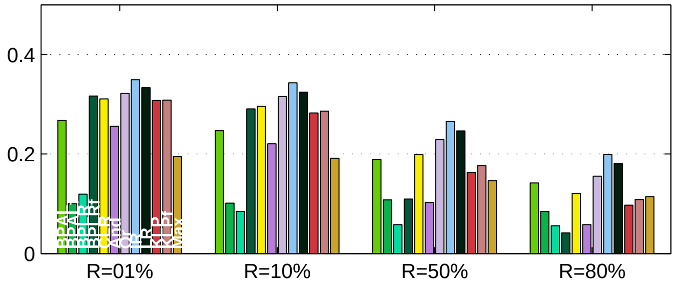

Figure S.18: **GO terms correctly found for a given protein for the Biological Process ontology (test set)** Average over proteins of the precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$.

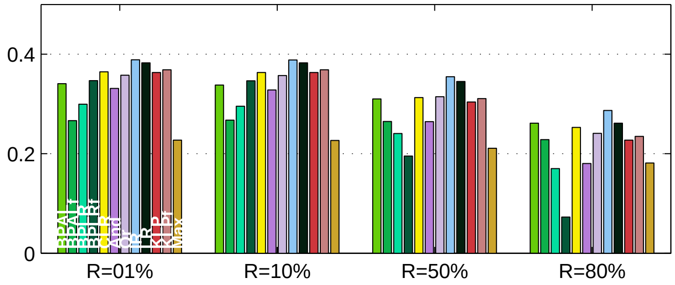

Figure S.19: **GO terms correctly found for a given protein for the Molecular Function ontology (hold-out set)** Average over proteins of the precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$.

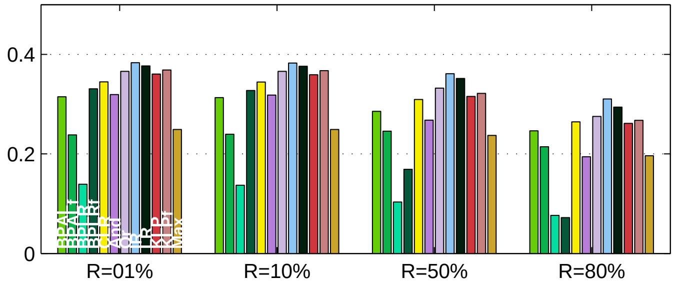

Figure S.20: **GO terms correctly found for a given protein for the Molecular Function ontology (test set)** Average over proteins of the precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$.

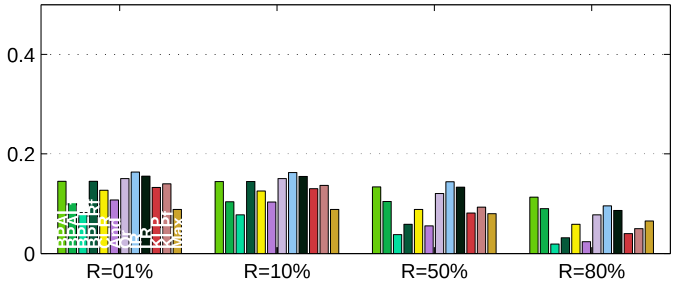

Figure S.21: **GO terms correctly found for a given protein for the Cellular Component ontology (hold-out set)** Average over proteins of the precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$.

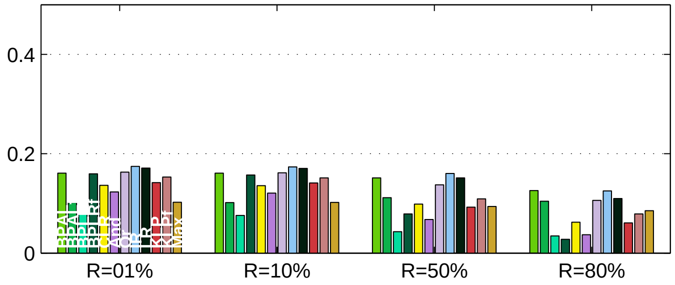

Figure S.22: **GO terms correctly found for a given protein for the Cellular Component ontology (test set)** Average over proteins of the precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$.

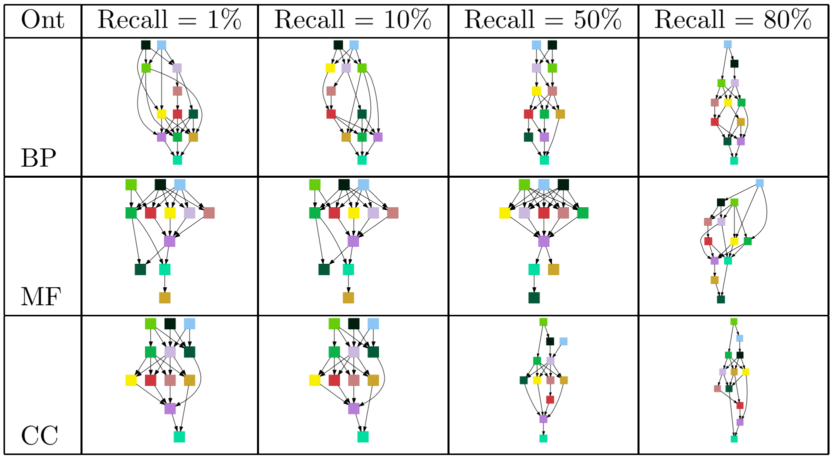

Figure S.23: **Statistical significance testing of per protein evaluation, irrespective of term size (hold-out set).** Each panel shows a directed graph in which nodes are methods and a directed edge from node A to node B indicates that method A performs significantly better than method B according to the Z-test.

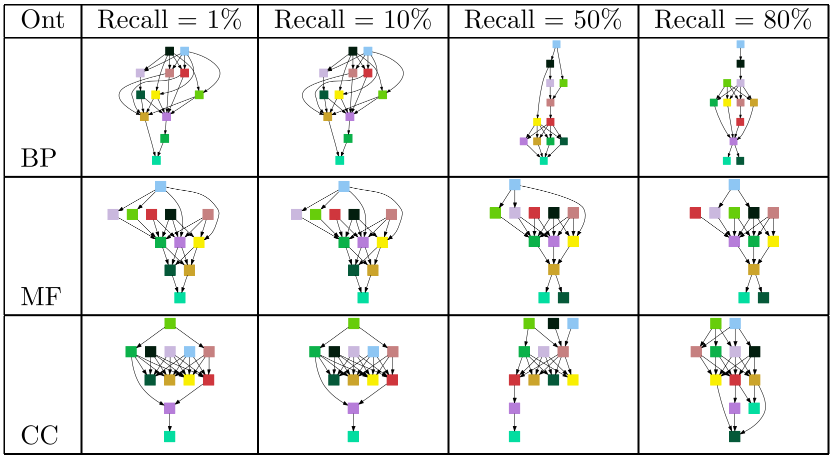

Figure S.24: **Statistical significance testing of per protein evaluation, irrespective of term size (test set).** Each panel shows a directed graph in which nodes are methods and a directed edge from node A to node B indicates that method A performs significantly better than method B according to the Z-test.

2.2 Directed graphs by ontology

2.3 Bar plots by ontology and term size

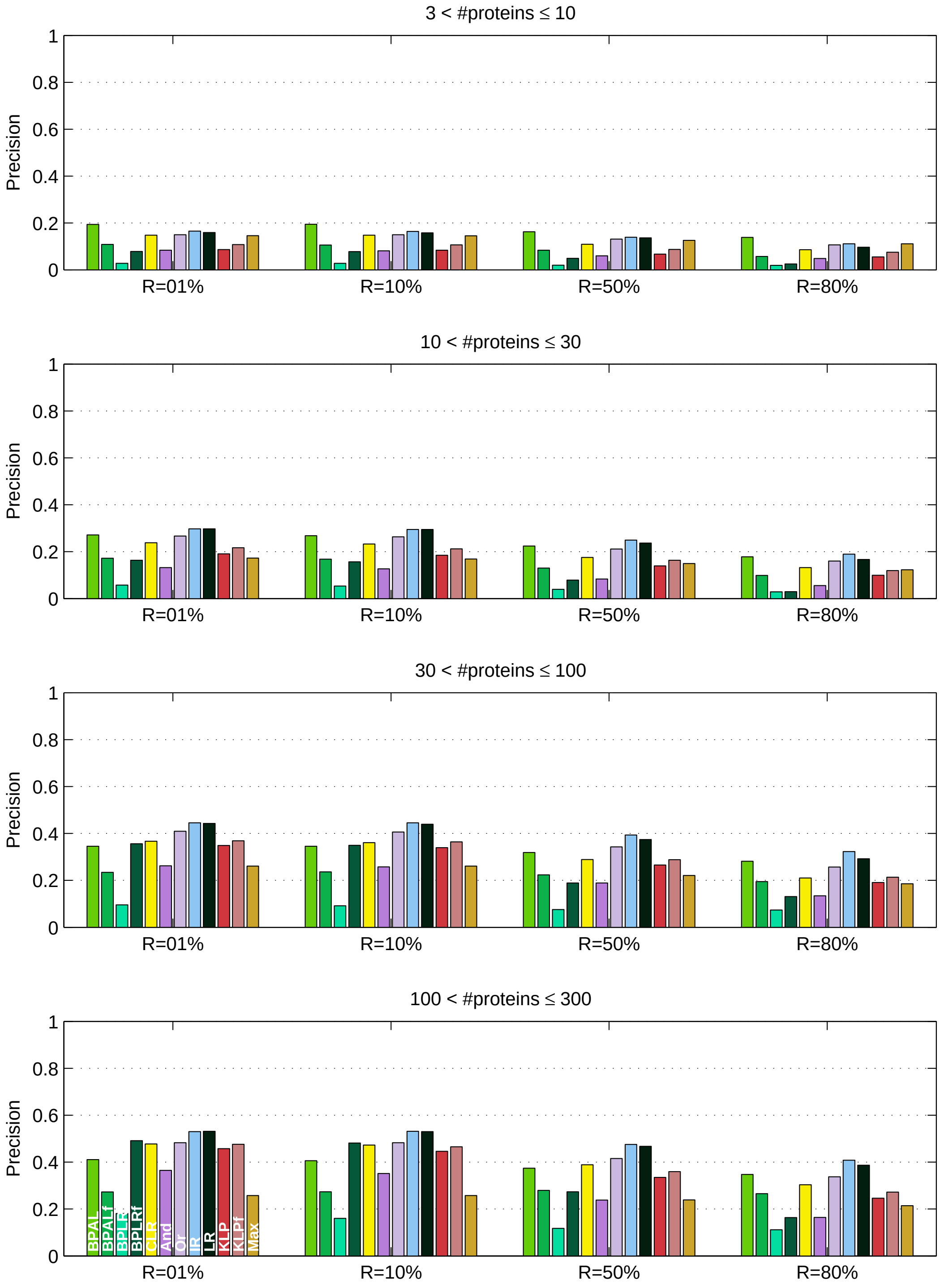

Figure S.25: **GO terms correctly found for a given protein for the Biological Process ontology (hold-out set)** Average over proteins of the precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$. Proteins are grouped according to how many terms are known for these proteins.

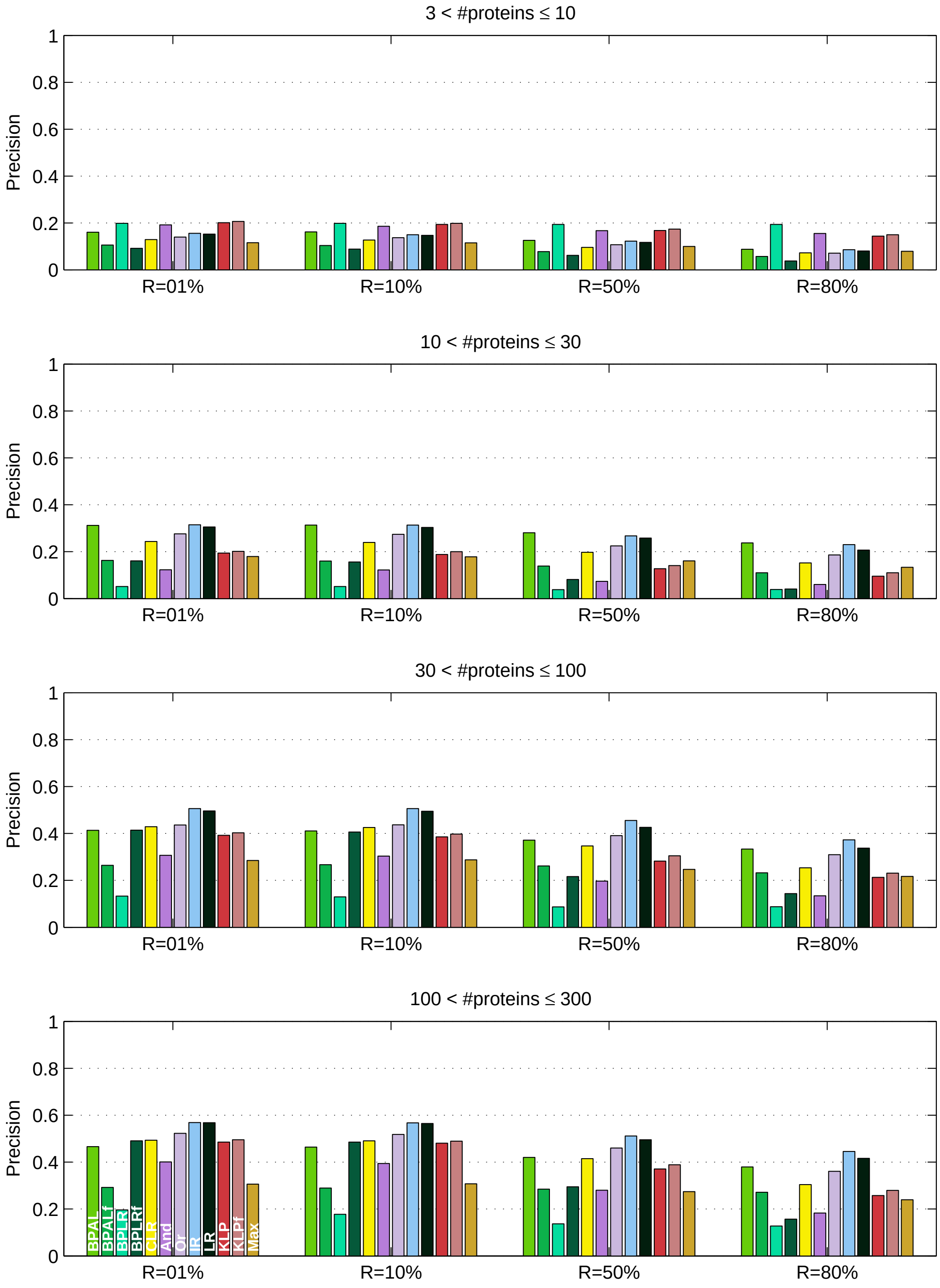

Figure S.26: **GO terms correctly found for a given protein for the Biological Process ontology (test set)** Average over proteins of the precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$. Proteins are grouped according to how many terms are known for these proteins.

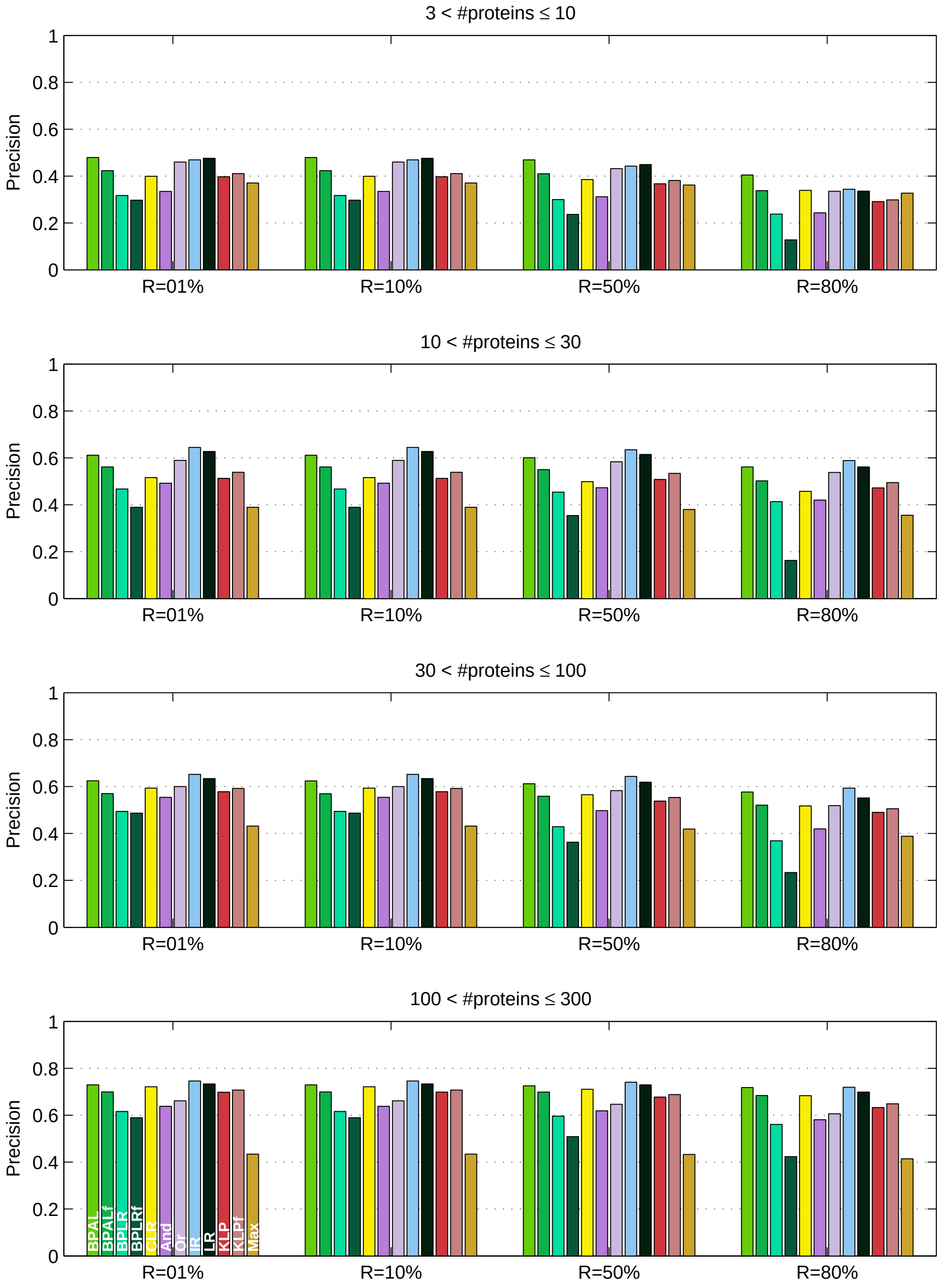

Figure S.27: **GO terms correctly found for a given protein for the Molecular Function ontology (hold-out set)** Average over proteins of the precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$. Proteins are grouped according to how many terms are known for these proteins.

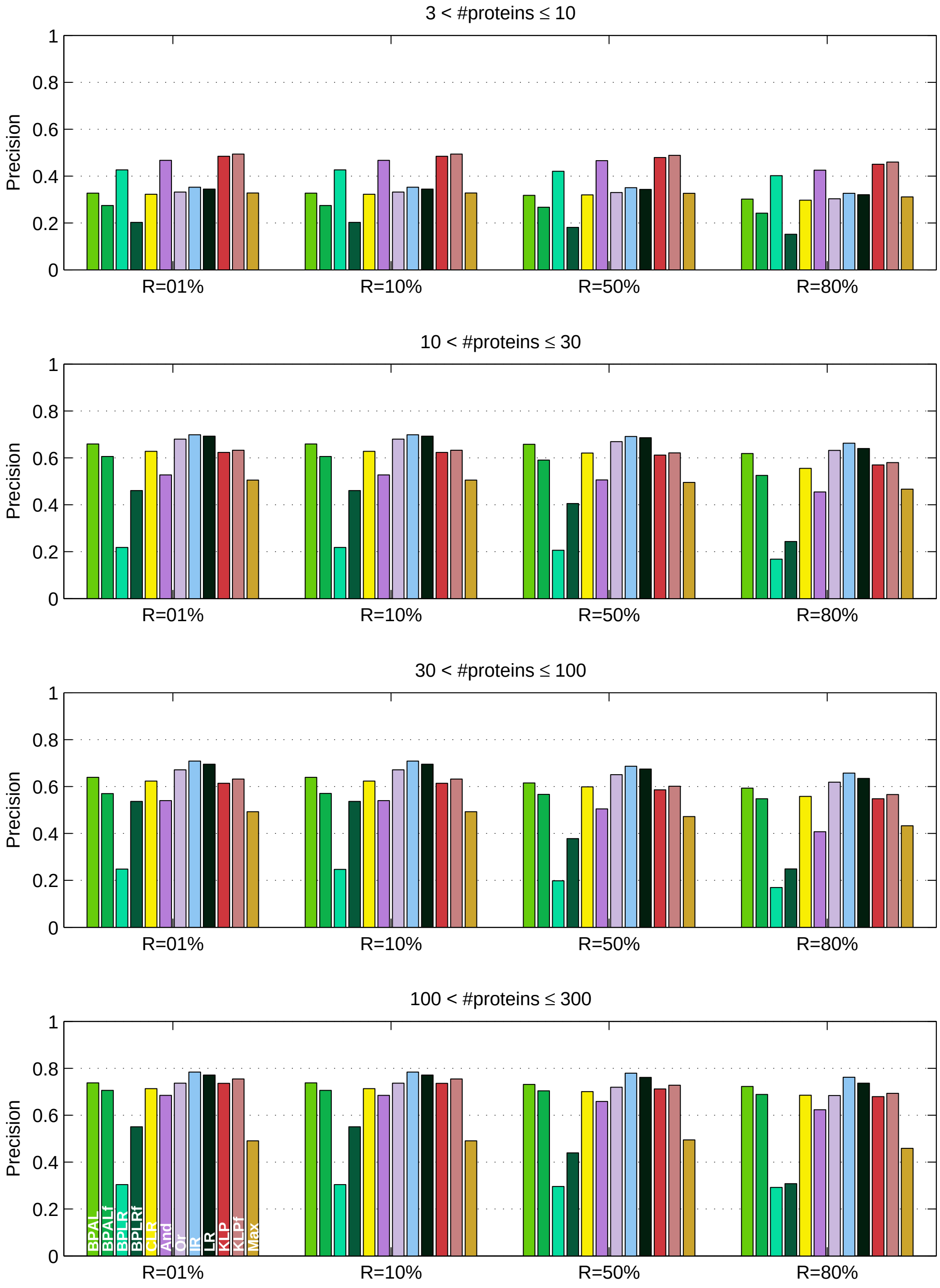

Figure S.28: **GO terms correctly found for a given protein for the Molecular Function ontology (test set)** Average over proteins of the precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$. Proteins are grouped according to how many terms are known for these proteins.

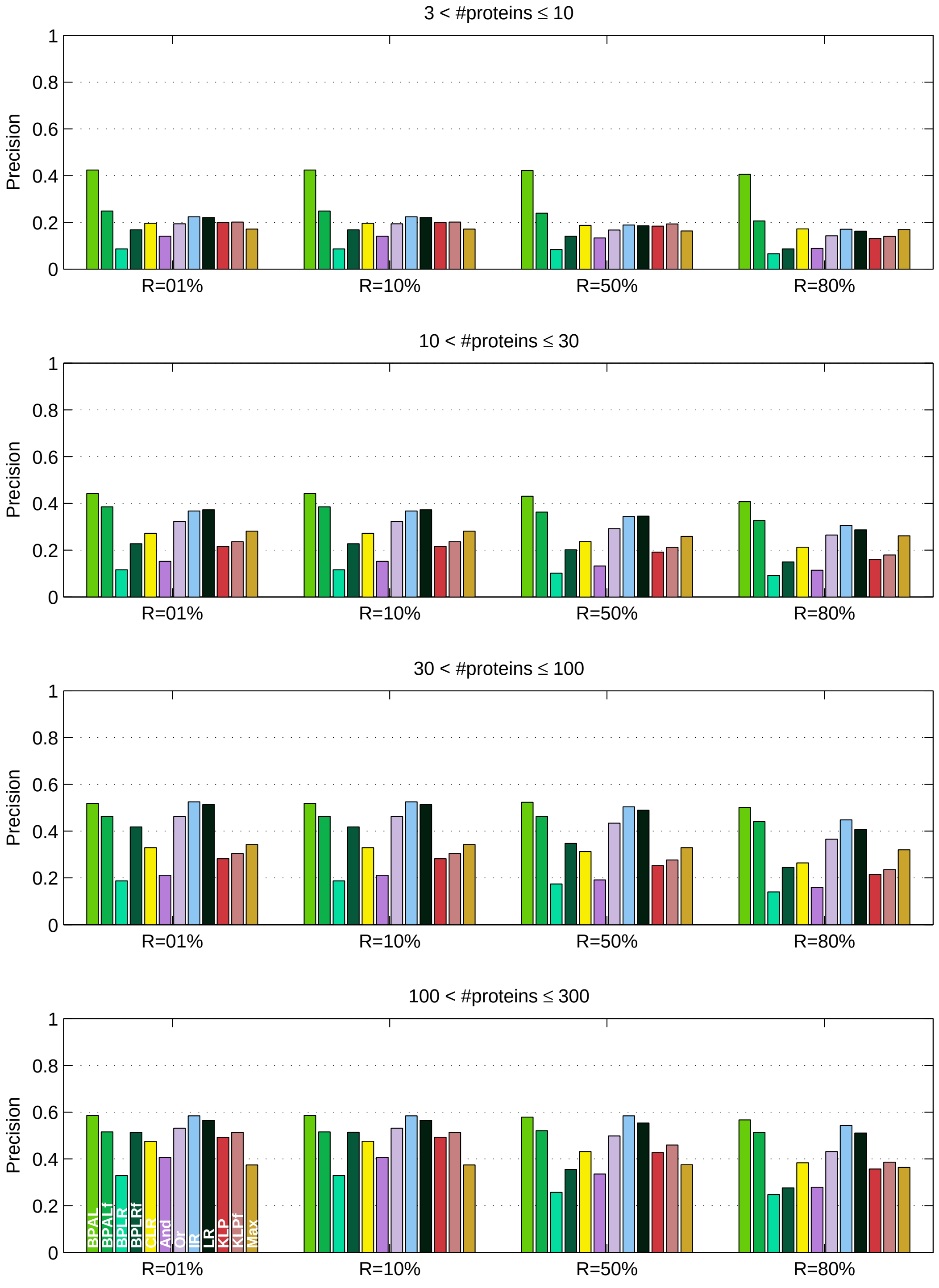

Figure S.29: **GO terms correctly found for a given protein for the Cellular Component ontology (hold-out set)** Average over proteins of the precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$. Proteins are grouped according to how many terms are known for these proteins.

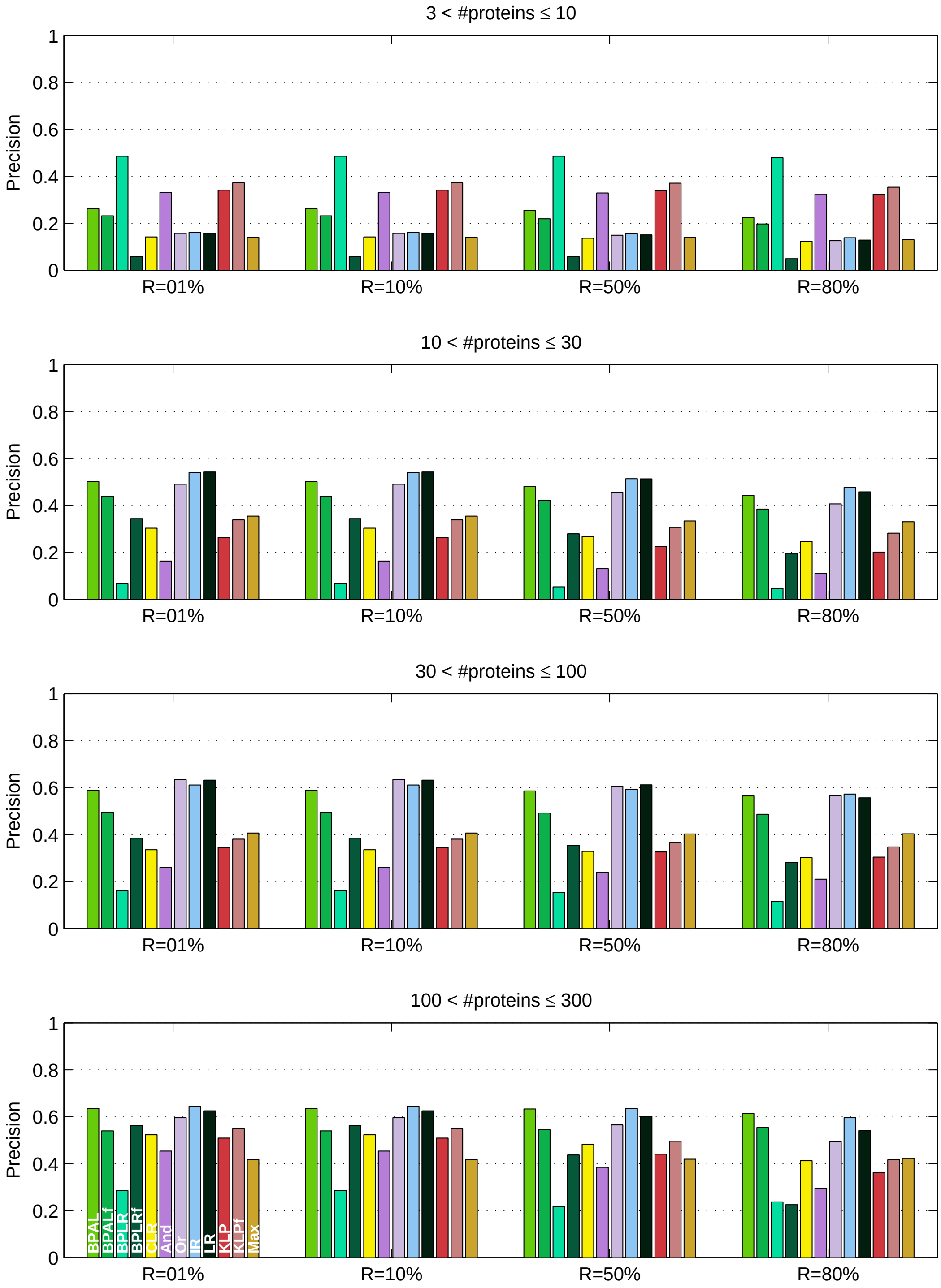

Figure S.30: **GO terms correctly found for a given protein for the Cellular Component ontology (test set)** Average over proteins of the precisions obtained by different methods for values of the recall respectively fixed at $R = 1\%$, $R = 10\%$, $R = 50\%$, $R = 80\%$. Proteins are grouped according to how many terms are known for these proteins.

2.4 Directed graphs by ontology and term size

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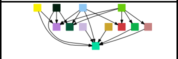
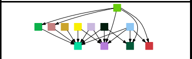
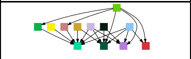
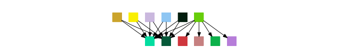
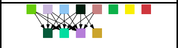
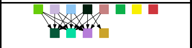
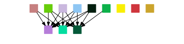
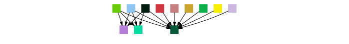
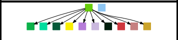
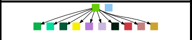
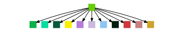
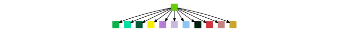
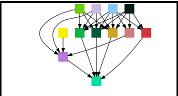
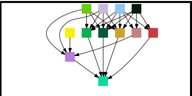
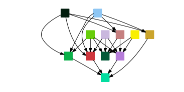
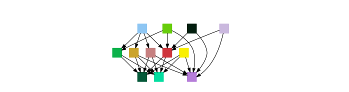
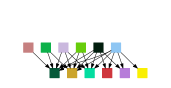
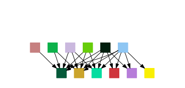
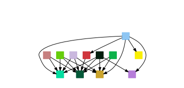
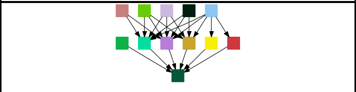
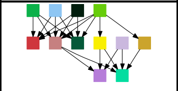
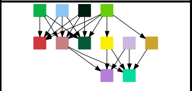
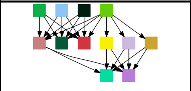
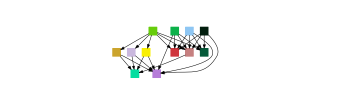
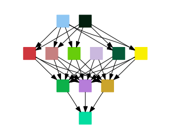
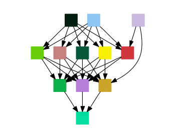
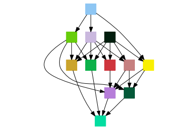
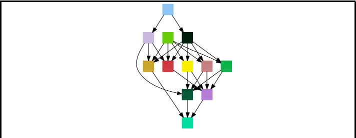
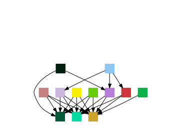
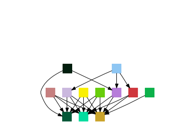
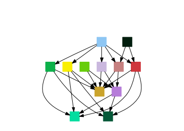
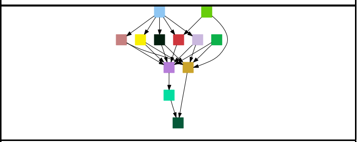
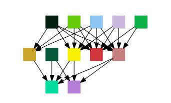
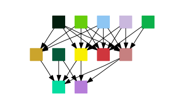
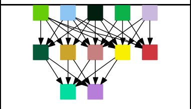
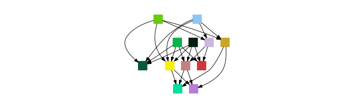
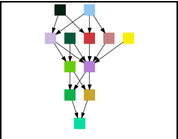
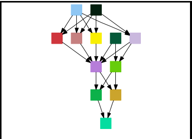
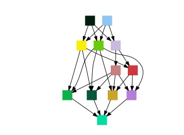
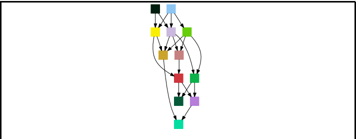
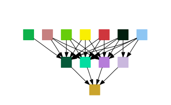
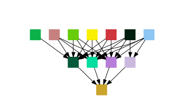
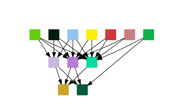
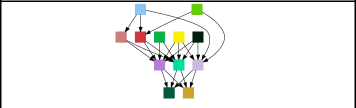
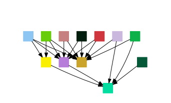
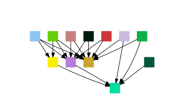
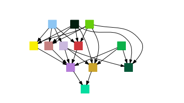
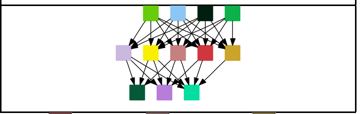
BP	3–10				
MF	3–10				
CC	3–10				
BP	11–30				
MF	11–30				
CC	11–30				
BP	31–100				
MF	31–100				
CC	31–100				
BP	101–300				
MF	101–300				
CC	101–300				

■ **BPAL** ■ **BPALf** ■ **BPLR** ■ **BPLRf** ■ **And** ■ **Or** ■ **IR** ■ **LR** ■ **KLP** ■ **KLPf** ■ **Max**

Figure S.31: **Statistical significance testing of per protein evaluation (hold-out set)** Each panel shows a directed graph in which nodes are methods and a directed edge from node A to node B indicates that method A performs significantly better than method B according to the Z-test.

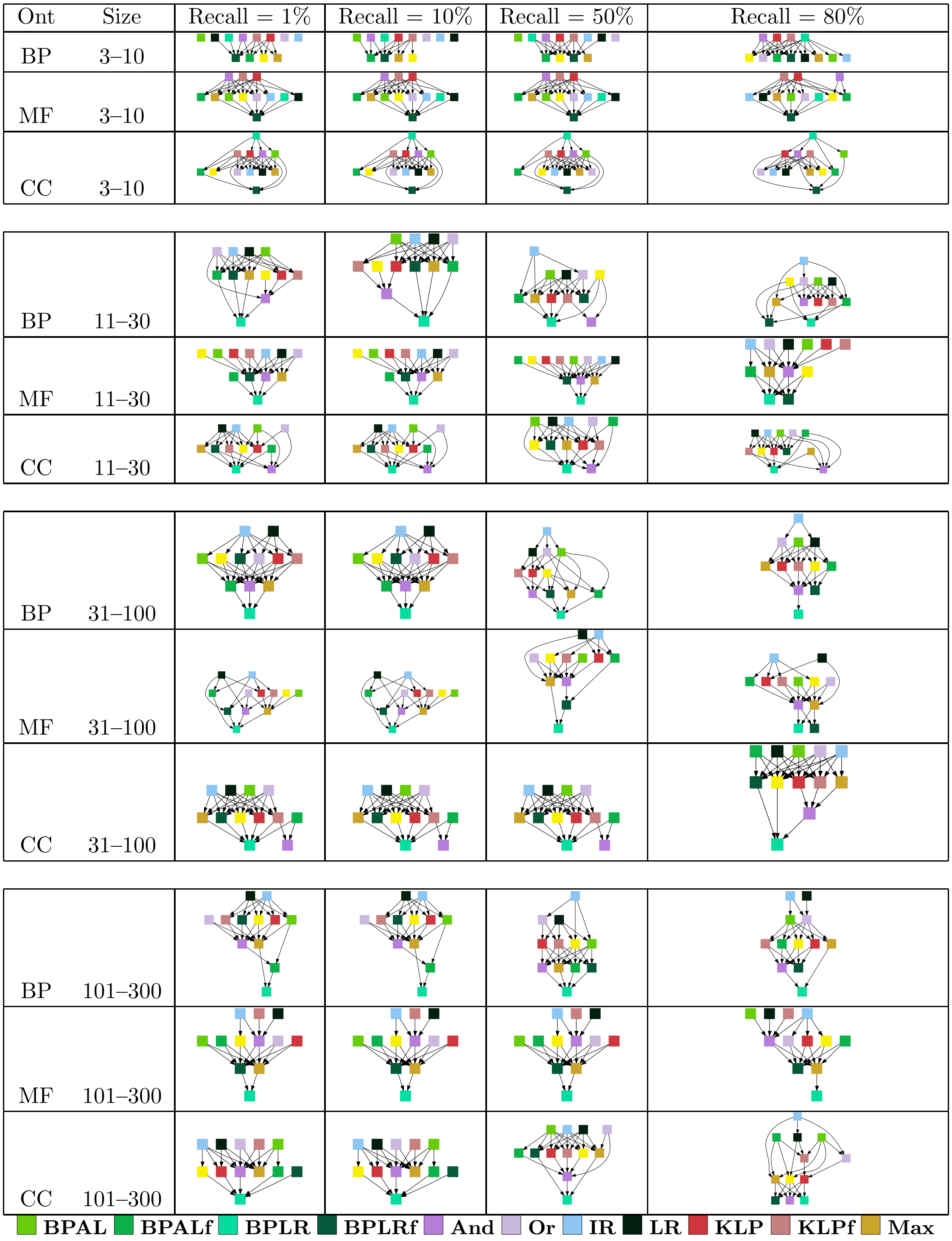


Figure S.32: **Statistical significance testing of per protein evaluation (test set)** Each panel shows a directed graph in which nodes are methods and a directed edge from node A to node B indicates that method A performs significantly better than method B according to the Z-test.

3 Joint annotation evaluation

3.1 Precision-recall curves by ontology

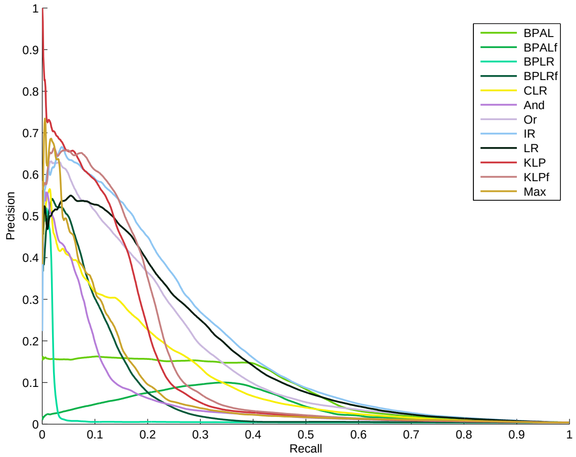


Figure S.33: **Precision-recall curve for joint annotation in the Biological Process ontology (hold-out set)** Precision-recall curve for the retrieval of valid (protein,term) pairs.

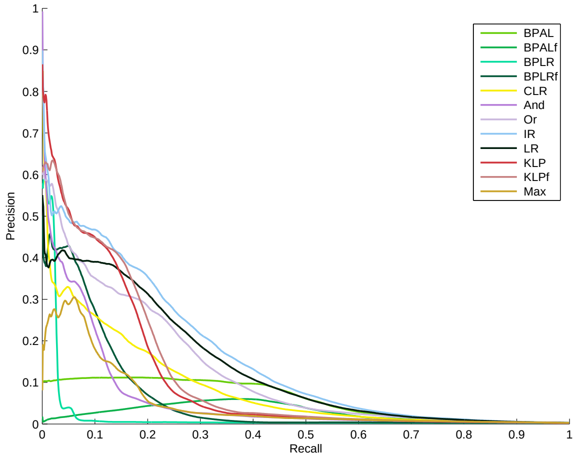


Figure S.34: **Precision-recall curve for joint annotation in the Biological Process ontology (test set)** Precision-recall curve for the retrieval of valid (protein,term) pairs.

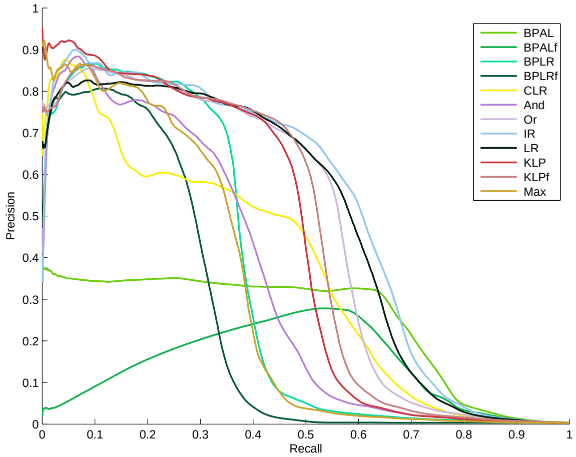


Figure S.35: **Precision-recall curve for joint annotation in the Molecular Function ontology (hold-out set)** Precision-recall curve for the retrieval of valid (protein,term) pairs.

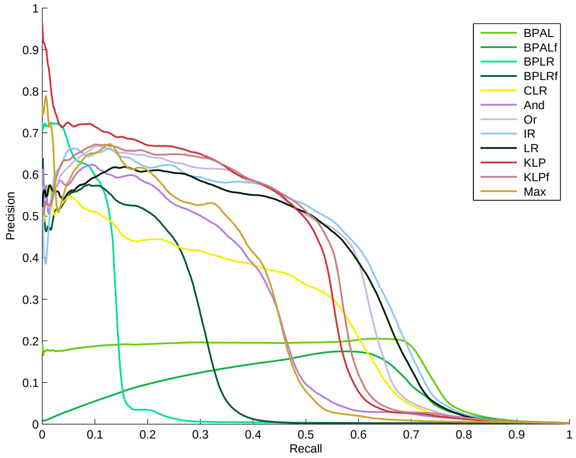


Figure S.36: **Precision-recall curve for joint annotation in the Molecular Function ontology (test set)** Precision-recall curve for the retrieval of valid (protein,term) pairs.

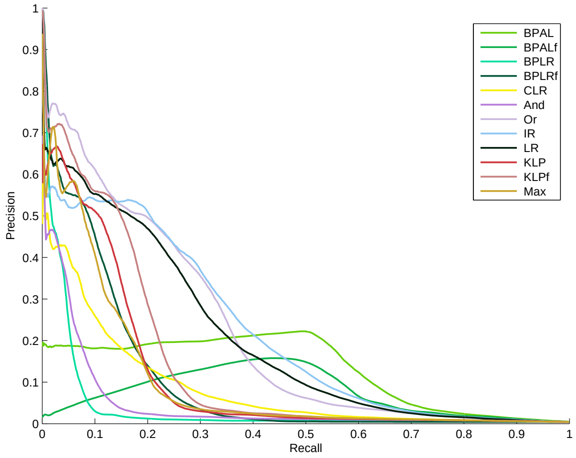


Figure S.37: **Precision-recall curve for joint annotation in the Cellular Component ontology (hold-out set)** Precision-recall curve for the retrieval of valid (protein,term) pairs.

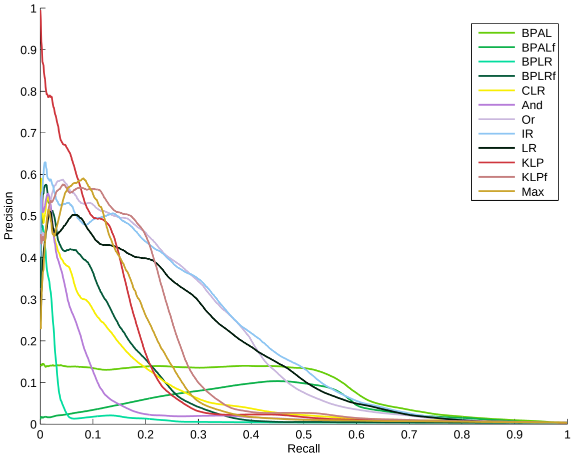


Figure S.38: **Precision-recall curve for joint annotation in the Cellular Component ontology (test set)** Precision-recall curve for the retrieval of valid (protein,term) pairs.

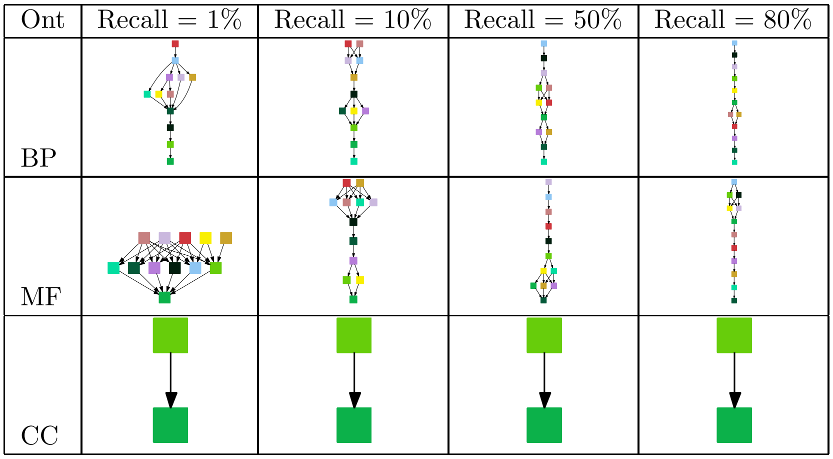


Figure S.39: **Statistical significance testing of joint evaluation, irrespective of term size (hold-out set).** Each panel shows a directed graph in which nodes are methods and a directed edge from node A to node B indicates that method A performs significantly better than method B according to the bootstrap test.

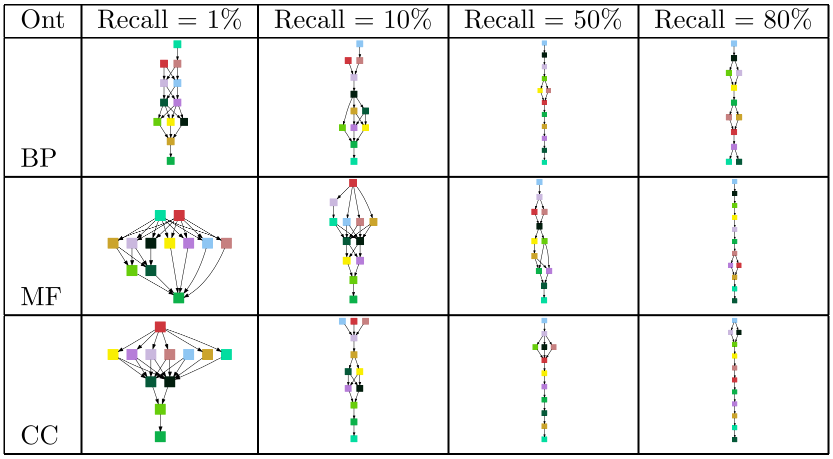


Figure S.40: **Statistical significance testing of joint evaluation, irrespective of term size (test set).** Each panel shows a directed graph in which nodes are methods and a directed edge from node A to node B indicates that method A performs significantly better than method B according to the bootstrap.

3.2 Directed graphs by ontology

3.3 Precision-recall curves by ontology and term size

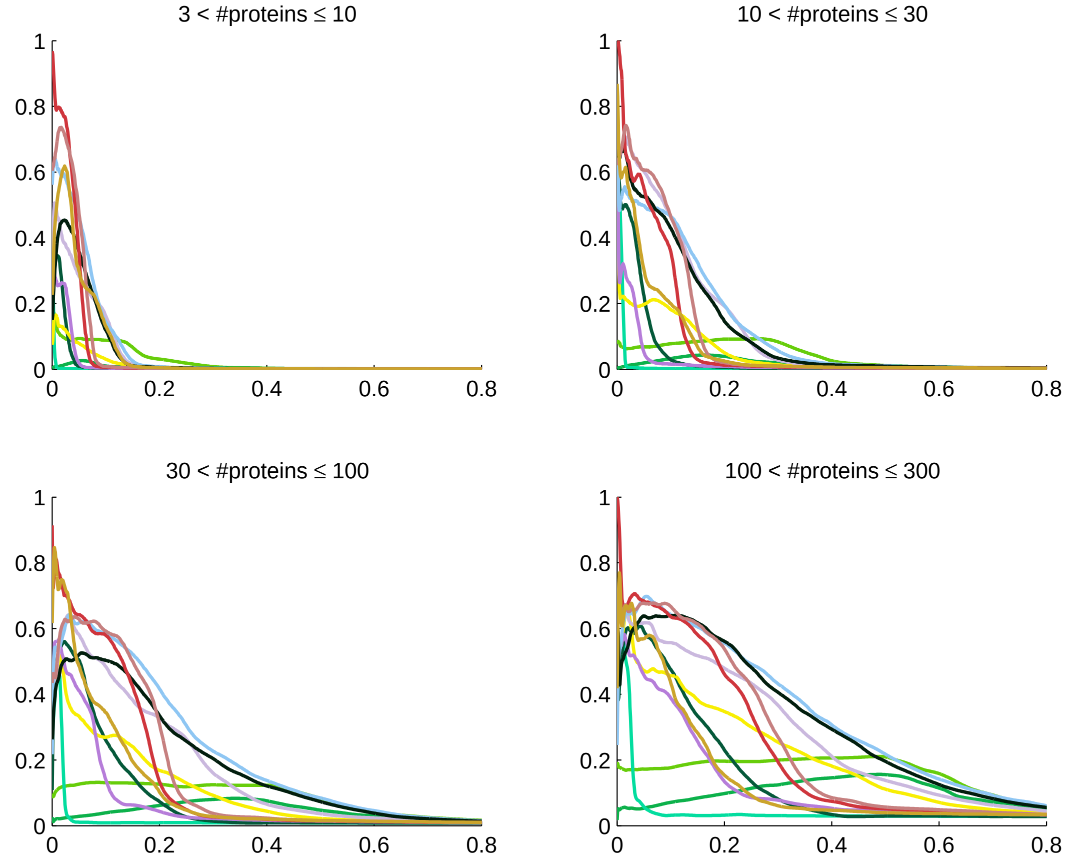


Figure S.41: **Precision-recall curves per size for joint annotation in the Biological Process ontology (hold-out set)** Precision-recall curve for 4 groups of terms with different levels of specificity in the ontology.

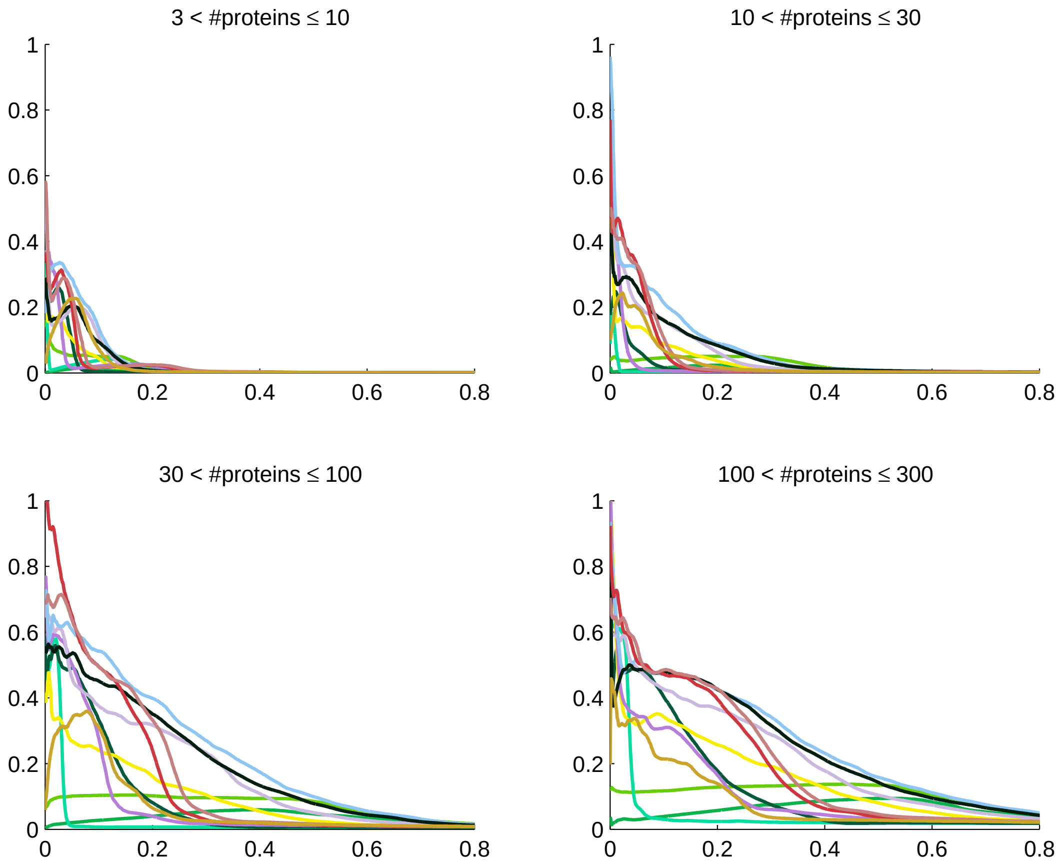


Figure S.42: **Precision-recall curves per size for joint annotation in the Biological Process ontology (test set)** Precision-recall curve for 4 groups of terms with different levels of specificity in the ontology.

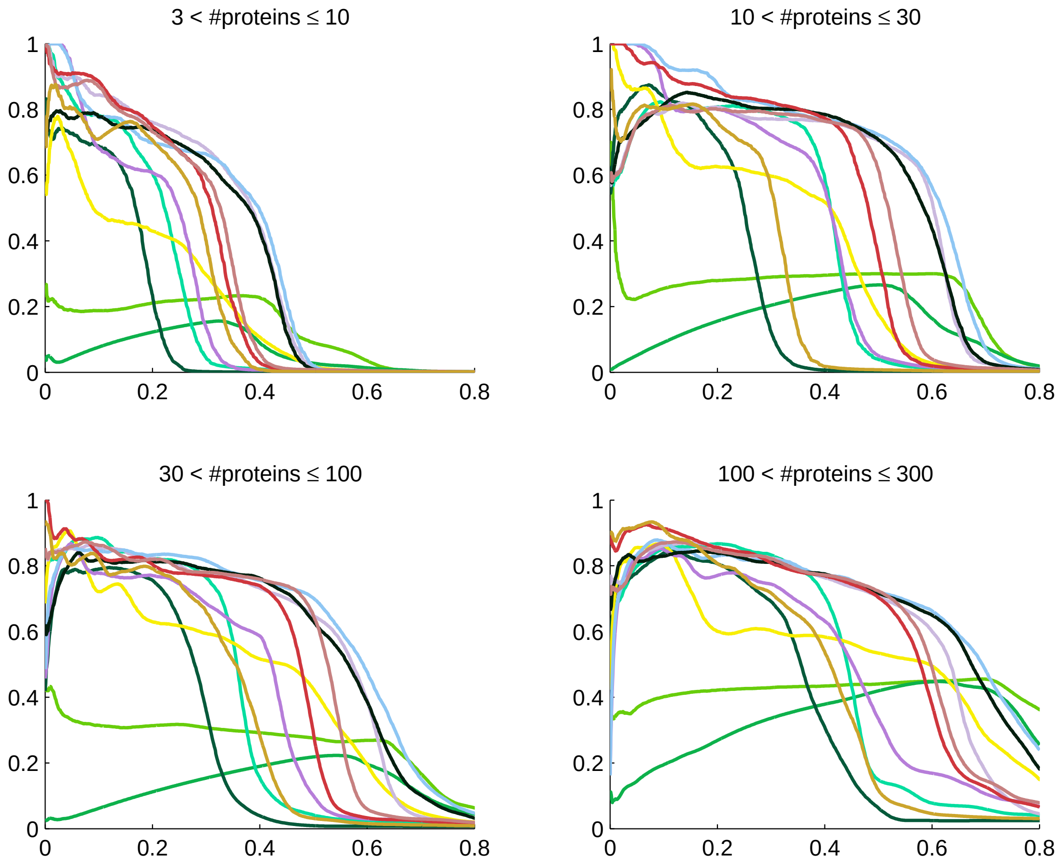


Figure S.43: **Precision-recall curves per size for joint annotation in the Molecular Function ontology (hold-out set)** Precision-recall curve for 4 groups of terms with different levels of specificity in the ontology.

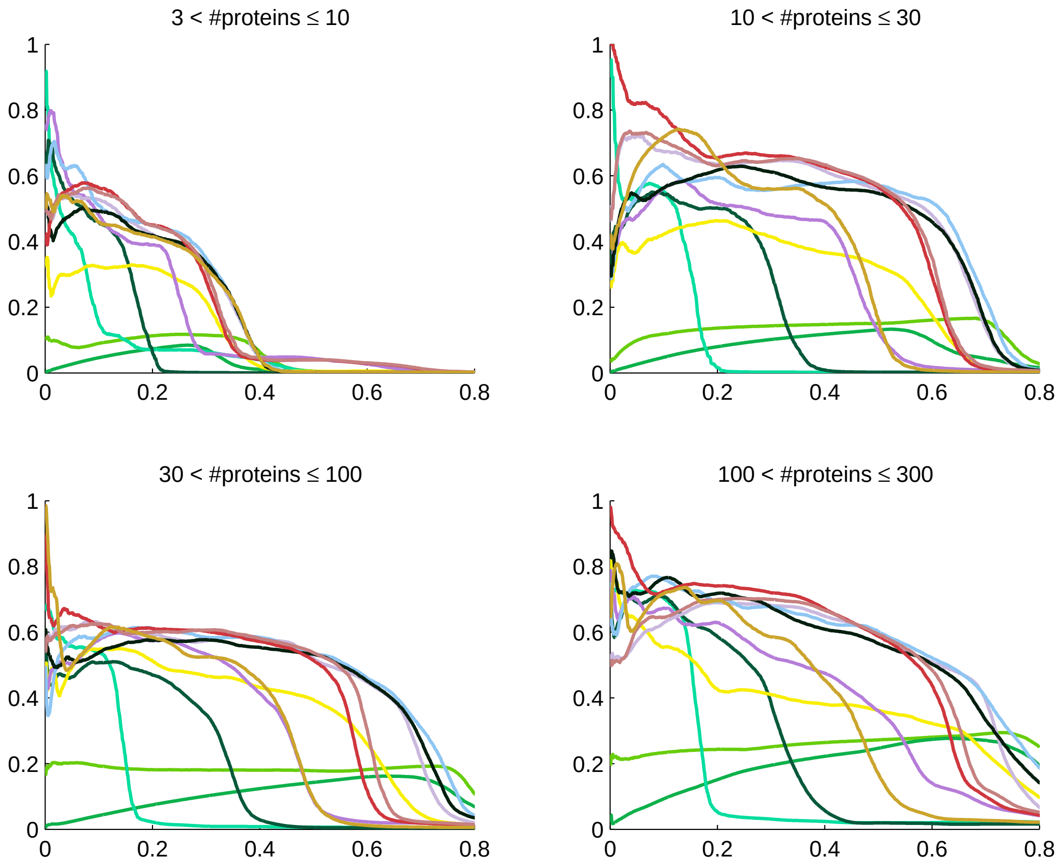


Figure S.44: **Precision-recall curves per size for joint annotation in the Molecular Function ontology (test set)** Precision-recall curve for 4 groups of terms with different levels of specificity in the ontology.

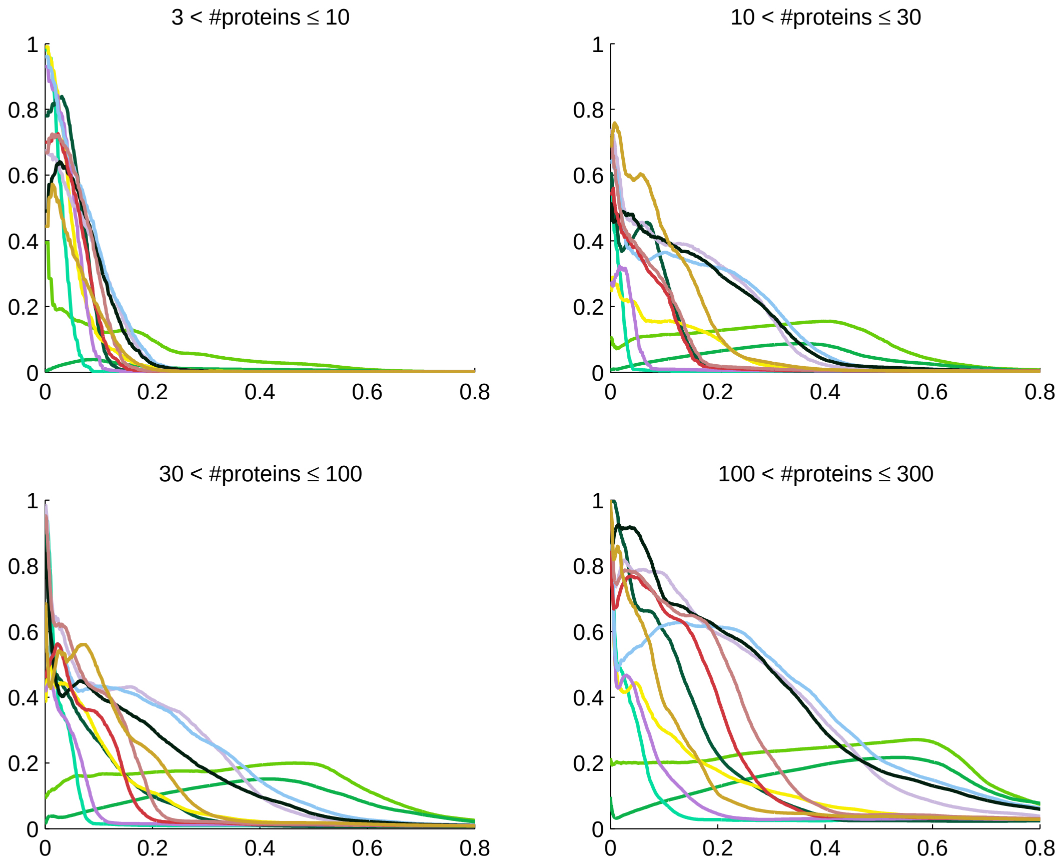


Figure S.45: **Precision-recall curves per size for joint annotation in the Cellular Component ontology (hold-out set)** Precision-recall curve for 4 groups of terms with different levels of specificity in the ontology.

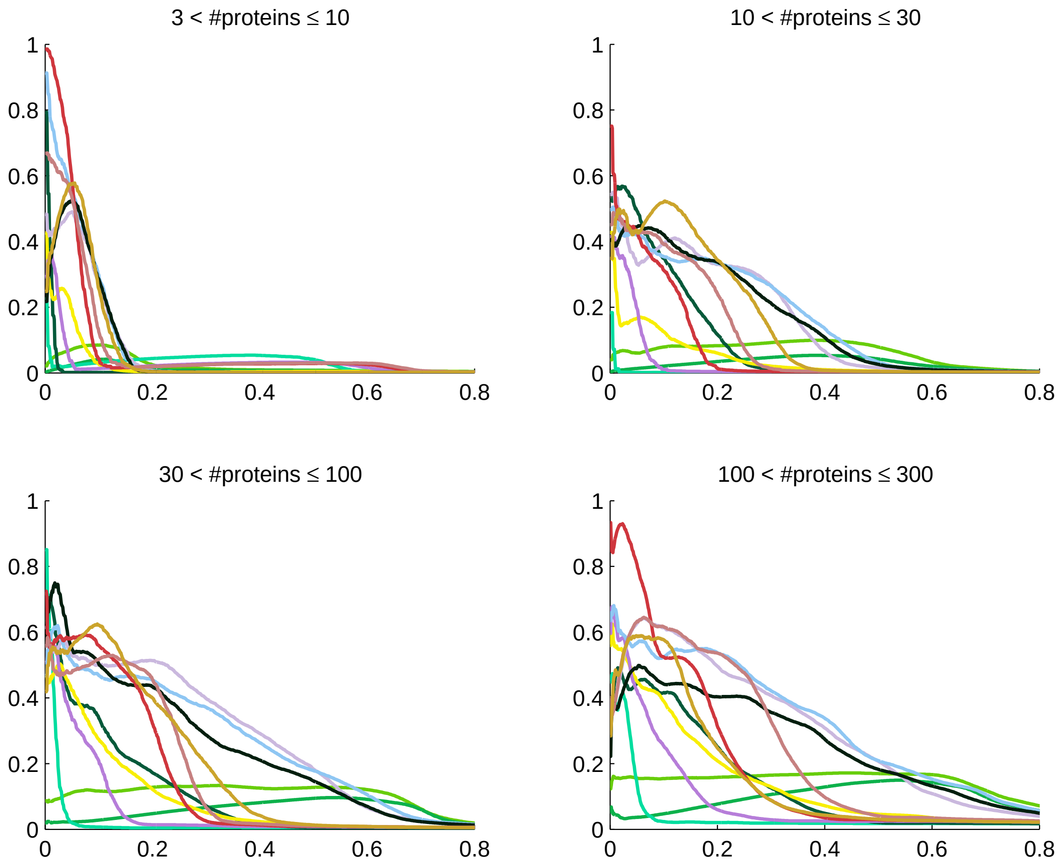
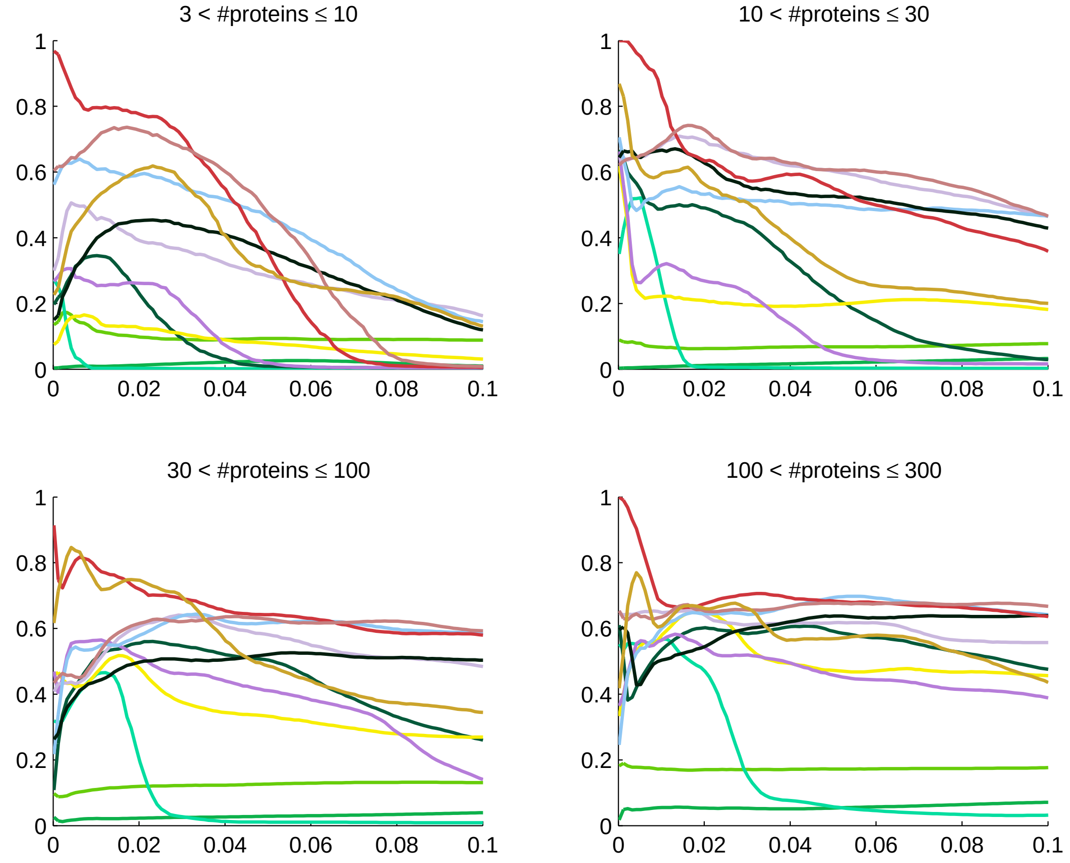


Figure S.46: **Precision-recall curves per size for joint annotation in the Cellular Component ontology (test set)** Precision-recall curve for 4 groups of terms with different levels of specificity in the ontology.

3.4 Zoomed precision-recall curves (recall $< 10\%$) by ontology and term size


3 < #proteins ≤ 10

10 < #proteins ≤ 30

30 < #proteins ≤ 100

100 < #proteins ≤ 300

Figure S.47: **Truncated precision-recall curves for joint annotation in the Biological Process ontology (hold-out set)** A zoom-in of the high precision regime of the previous plot.

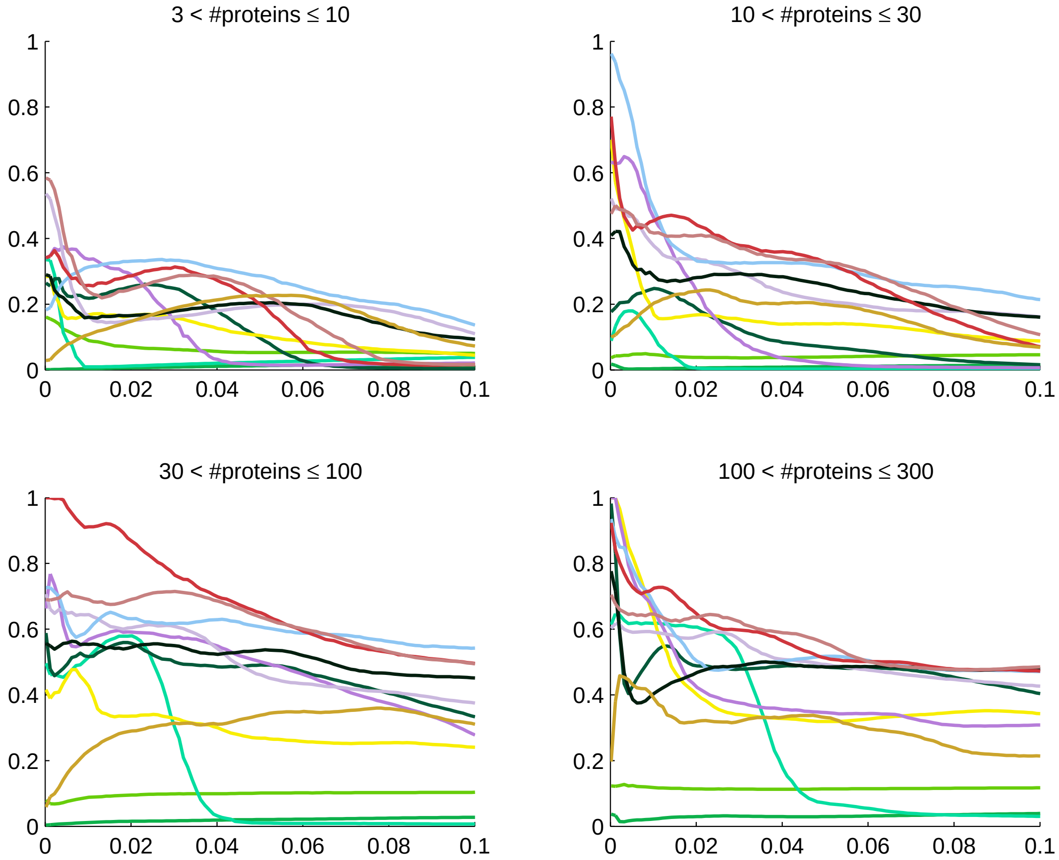


Figure S.48: **Truncated precision-recall curves for joint annotation in the Biological Process ontology (test set)** A zoom-in of the high precision regime of the previous plot.

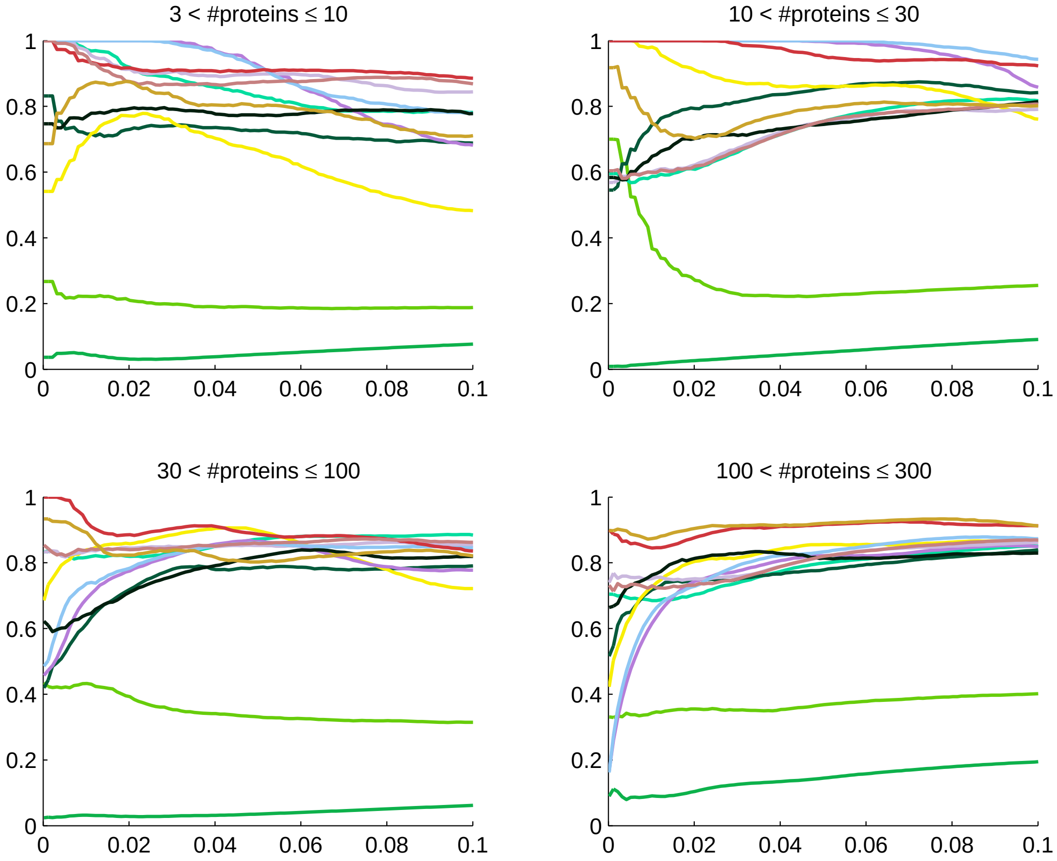


Figure S.49: **Truncated precision-recall curves for joint annotation in the Molecular Function ontology (hold-out set)** A zoom-in of the high precision regime of the previous plot.

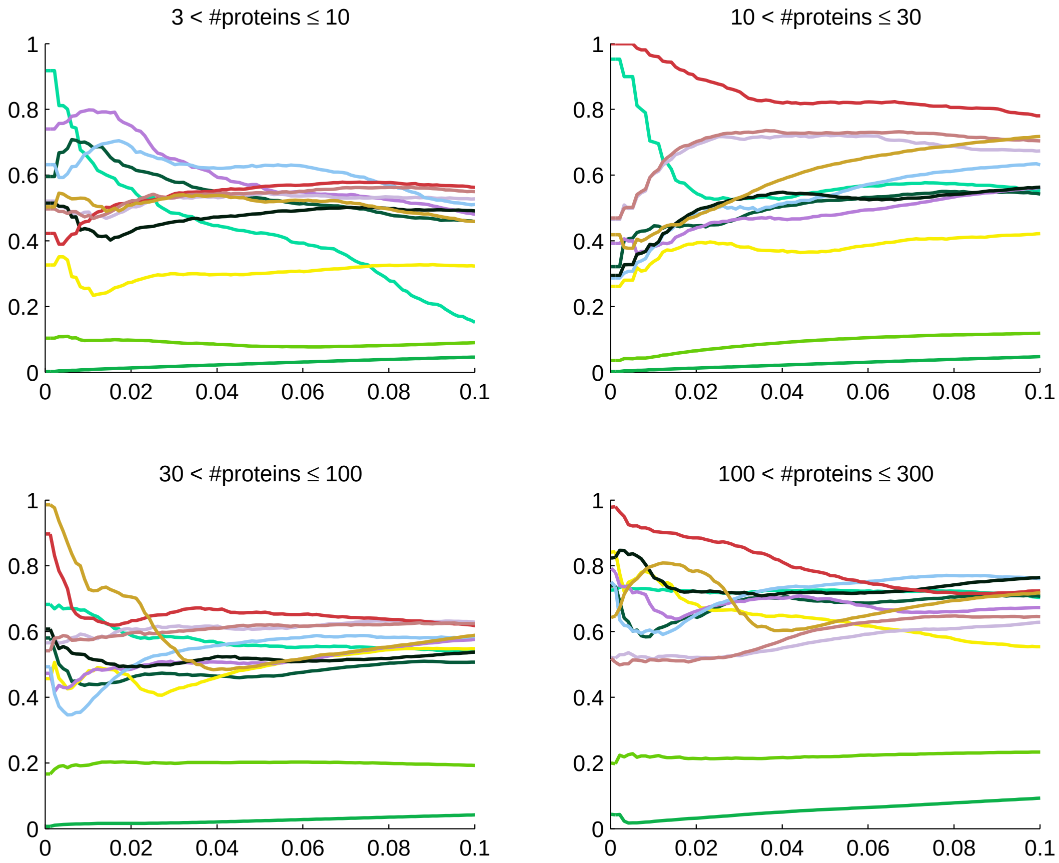


Figure S.50: **Truncated precision-recall curves for joint annotation in the Molecular Function ontology (test set)** A zoom-in of the high precision regime of the previous plot.

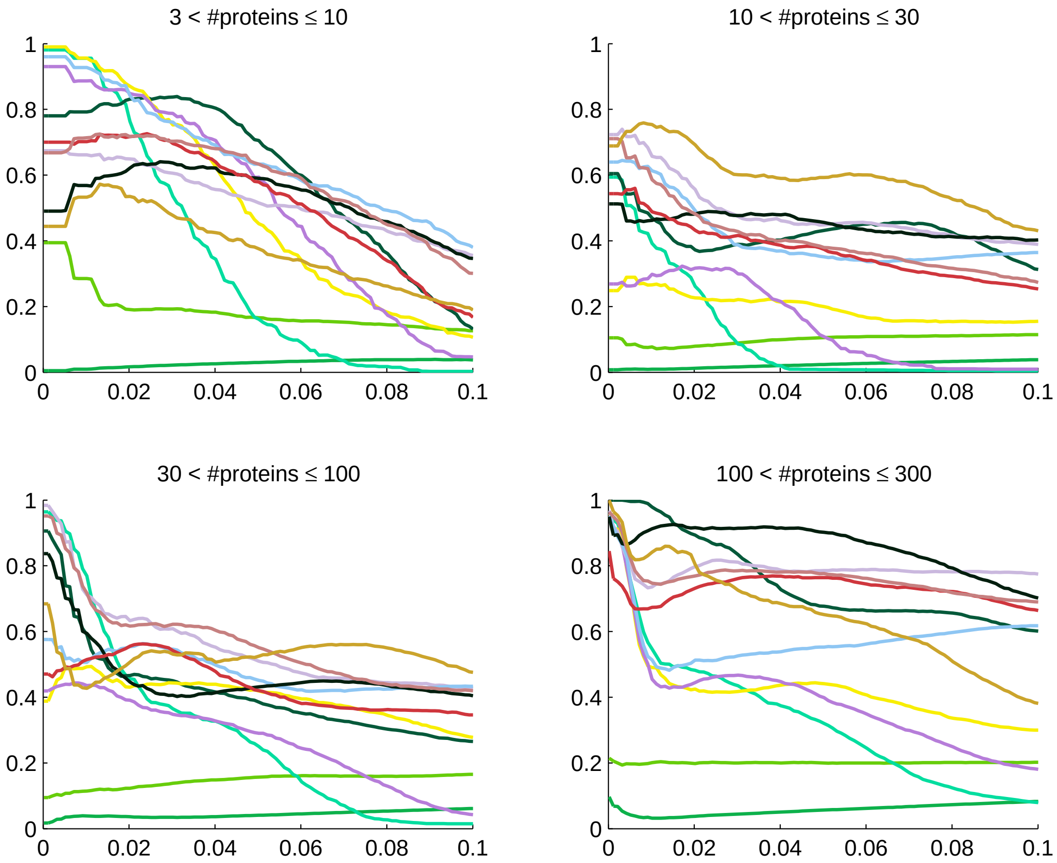


Figure S.51: **Truncated precision-recall curves for joint annotation in the Cellular Component ontology (hold-out set)** A zoom-in of the high precision regime of the previous plot.

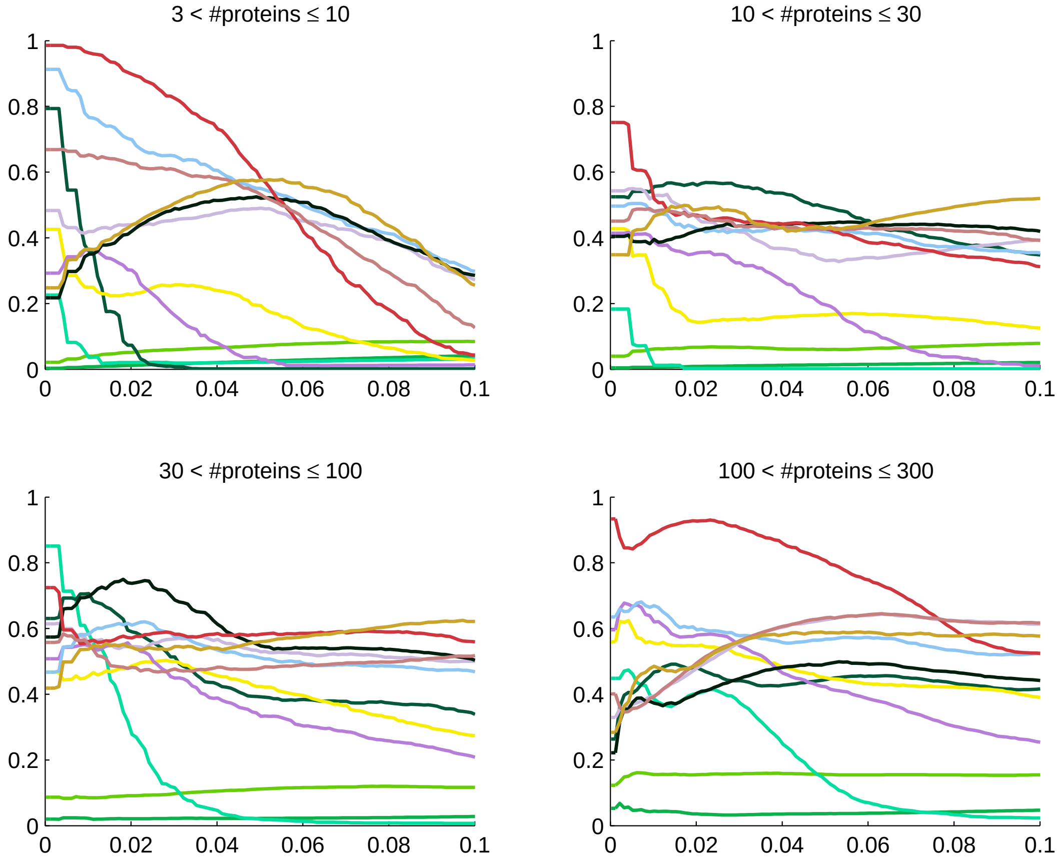


Figure S.52: **Truncated precision-recall curves for joint annotation in the Cellular Component ontology (test set)** A zoom-in of the high precision regime of the previous plot.

3.5 Directed graphs by ontology and term size

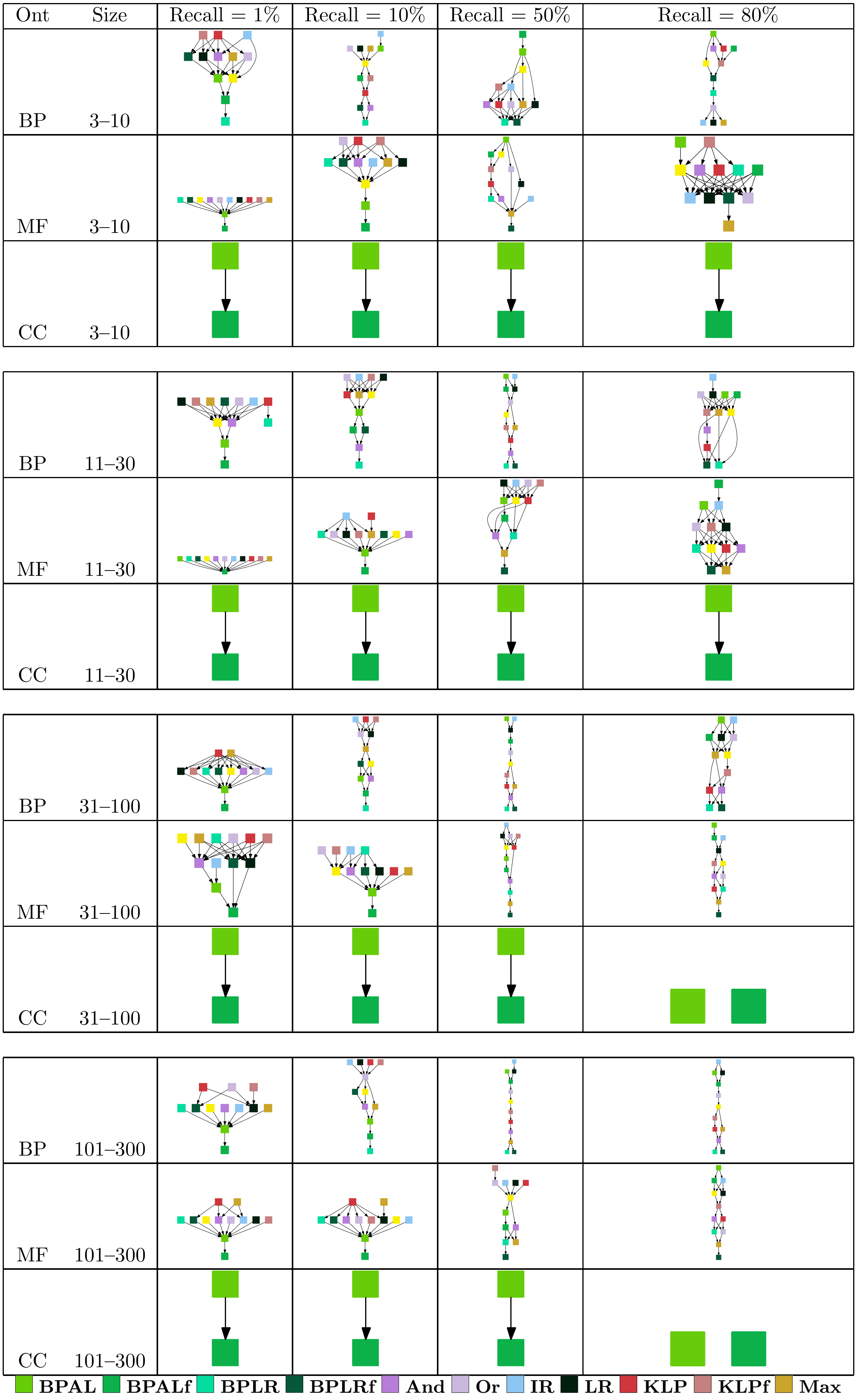


Figure S.53: **Statistical significance testing of joint evaluation (hold-out set)** Each panel shows a directed graph in which nodes are methods and a directed edge from node A to node B indicates that method A performs significantly better than method B according to the bootstrap test.

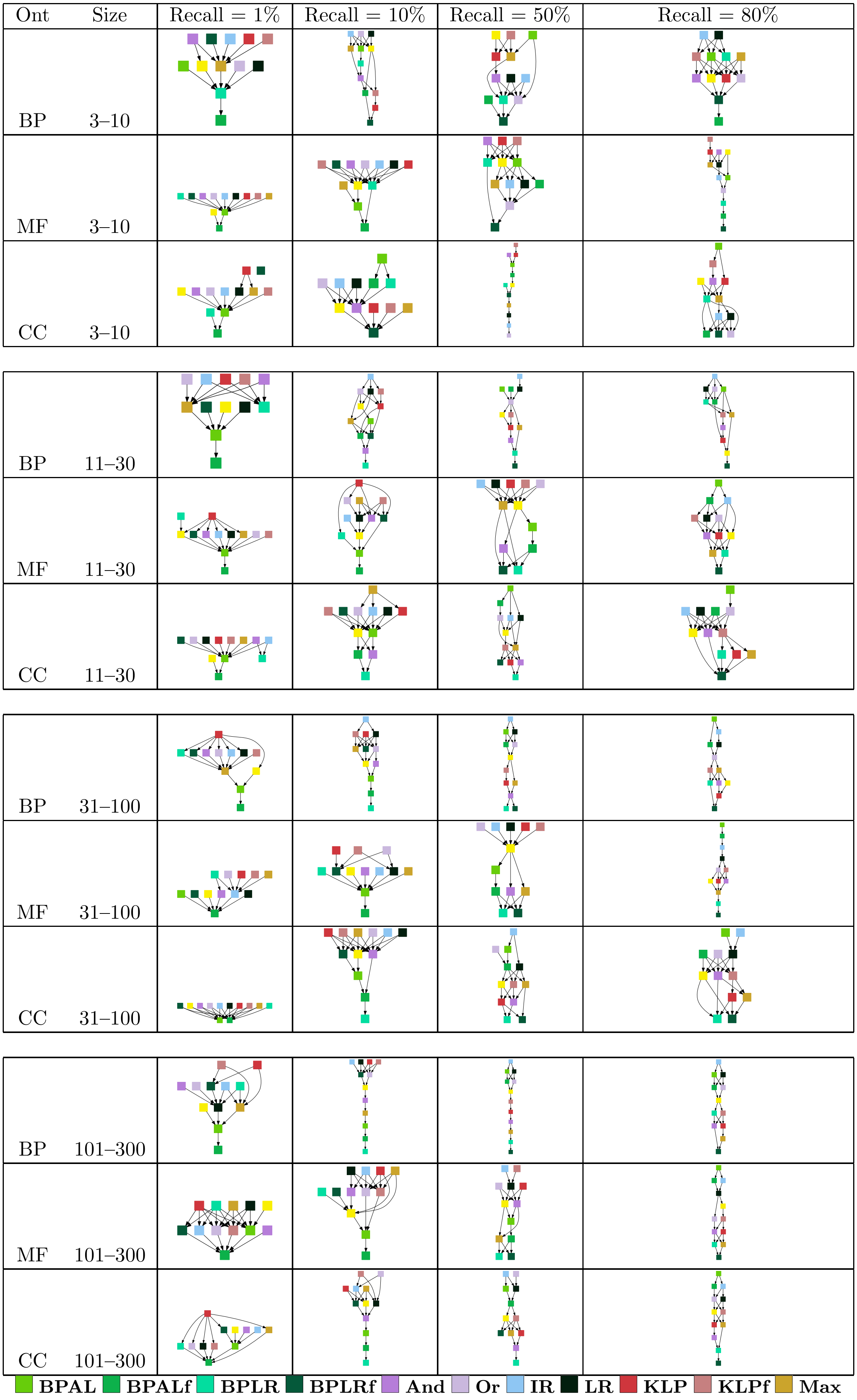


Figure S.54: **Statistical significance testing of joint evaluation (test set)** Each panel shows a directed graph in which nodes are methods and a directed edge from node A to node B indicates that method A performs significantly better than method B according to the bootstrap test.