CAID-vect

February 5, 2020

IMPORTANT: * dataset: new-disprot_all_simple: * new: last round annotations * disprot: disorder comes from disprot annotations * all: no filtering by method (xray, nmr...) * simple: residues falling out of disprot annotations are considered ordered * threshold: default * baselines: * random: completely random * suffledataset: random shuffling at dataset level (disorder content maintaned at dataset level) * shuffletarget: random shuffling at protein level (disorder content maintaned at protein level) * new-disprot-all_simple_cons: naive predictor based on the opposite of conservation * new-disprot-pdb-r_simple: what is not on pdb is disorder

0.1 Metrics tables

- bac: balanced accuracy,
- csi: critical score index / threat score,
- f05: f 0.5 score
- f1s: f 1 score / f score,
- f2s: f 2 score
- fnr: false negative rate / miss-rate
- fom: false omission rate'
- fpr: false postive rate / fall-out
- inf: informedness / bookmaker informedness
- mcc: matthew's correlation coefficient
- mk: markedness
- npv: negative predictive value
- ppv: precision / positive predictive value
- tnr: true negative rate / specificity / selectivity
- tpr: true positive rate / sensitivity / recall
- aucroc: area under the ROC curve
- aucpr aurea under the Precision-Recall curve
- aps: average precision score
- thr: prediction score cutoff

0.1.1 Metrics calculated at dataset level

	bac	csi	f05	f1s	f2s	fnr	fom	\
D029_SPOT-Disorder2	0.720	0.306	0.381	0.469	0.608	0.241	0.071	
D013_fIDPln	0.679	0.287	0.417	0.446	0.480	0.494	0.101	
D014 fIDPnn	0.626	0.241	0.470	0.388	0.330	0.700	0.124	

```
D025_RawMSA
                              0.709
                                     0.285
                                             0.365
                                                    0.444
                                                            0.567
                                                                   0.304
                                                                          0.075
                              0.707
                                      0.274
                                                    0.430
                                                                   0.252
D028_SP0T-Disorder1
                                             0.343
                                                            0.577
                                                                          0.068
D026_AUCpreD
                              0.696
                                     0.276
                                             0.354
                                                    0.433
                                                            0.556
                                                                   0.313
                                                                          0.081
                                      0.264
D002_Predisorder
                              0.695
                                             0.324
                                                    0.418
                                                            0.588
                                                                   0.193
                                                                          0.063
D018_ESpritz-D
                              0.632
                                     0.242
                                             0.417
                                                    0.390
                                                            0.366
                                                                   0.648
                                                                          0.121
                                     0.260
D008_IsUnstruct
                              0.692
                                             0.325
                                                    0.413
                                                            0.565
                                                                   0.252
                                                                          0.071
D005 IUPred-long
                                     0.264
                                             0.345
                                                    0.418
                                                            0.530
                                                                   0.355
                                                                          0.087
                              0.683
                                     0.265
D027_AUCpreD-np
                              0.674
                                             0.360
                                                    0.418
                                                            0.499
                                                                   0.427
                                                                          0.096
                                                                   0.366
D003 IUPred2A-long
                                     0.263
                                                    0.415
                              0.680
                                             0.344
                                                            0.524
                                                                          0.089
D021 MobiDB-lite
                              0.690
                                     0.256
                                             0.318
                                                    0.407
                                                            0.565
                                                                   0.239
                                                                          0.070
D030 SPOT-Disorder-Single
                                     0.261
                                                    0.414
                                                                   0.443
                              0.668
                                             0.358
                                                            0.489
                                                                          0.099
D004_IUPred2A-short
                              0.669
                                     0.261
                                             0.357
                                                    0.414
                                                            0.492
                                                                   0.437
                                                                          0.098
D024 DisoMine
                              0.670
                                     0.260
                                             0.353
                                                    0.413
                                                            0.497
                                                                   0.425
                                                                          0.097
D006_IUPred-short
                              0.668
                                     0.259
                                             0.354
                                                    0.411
                                                            0.490
                                                                   0.438
                                                                          0.099
D015 VSL2B
                                     0.243
                                             0.298
                                                    0.391
                                                            0.568
                                                                   0.185
                              0.680
                                                                          0.061
D020_ESpritz-X
                              0.658
                                     0.252
                                             0.351
                                                    0.403
                                                            0.471
                                                                   0.468
                                                                          0.103
                                     0.245
                                                    0.394
                                                            0.548
                                                                   0.259
DO31_JRONN
                              0.675
                                             0.307
                                                                          0.076
D019_ESpritz-N
                              0.670
                                     0.246
                                             0.315
                                                    0.395
                                                            0.530
                                                                   0.313
                                                                          0.085
                                     0.227
                                                    0.000
                                                                   1.000
shuffletargets
                              0.624
                                             0.000
                                                            0.000
                                                                          0.122
D011_DISOPRED-3.1
                              0.659
                                     0.240
                                             0.312
                                                    0.387
                                                            0.510
                                                                   0.353
                                                                          0.092
                                     0.239
                                             0.308
                                                    0.385
                                                                   0.341
D001_PyHCA
                              0.659
                                                            0.513
                                                                          0.091
new-pdb-r simple
                              0.631
                                     0.208
                                             0.251
                                                    0.345
                                                            0.555
                                                                   0.069
                                                                          0.039
D007 FoldUnfold
                              0.642
                                     0.223
                                             0.287
                                                    0.365
                                                            0.500
                                                                   0.334
                                                                          0.094
D017 DisEMBL-465
                                     0.209
                                             0.325
                                                    0.346
                                                                   0.613 0.124
                              0.612
                                                            0.370
D016 DisEMBL-HL
                              0.605
                                     0.199
                                             0.272
                                                    0.332
                                                            0.428
                                                                   0.470 0.118
D010 DisPredict-2
                              0.588
                                     0.186
                                             0.274
                                                    0.314
                                                            0.368
                                                                   0.584 0.129
D023 S2D-2
                                                                   0.062 0.055
                              0.573
                                     0.184
                                             0.222
                                                    0.310
                                                            0.519
D022 S2D-1
                              0.571
                                     0.183
                                             0.221
                                                    0.310
                                                            0.515
                                                                   0.075 0.063
D009_GlobPlot
                              0.569
                                     0.180
                                             0.225
                                                    0.304
                                                            0.469
                                                                   0.265
                                                                          0.113
                                     0.162
                                             0.244
                                                    0.278
                                                            0.325
                                                                   0.635
D033_DynaMine
                              0.561
                                                                          0.140
new-disprot-all_simple_cons
                              0.522
                                     0.166
                                             0.202
                                                    0.285
                                                            0.486
                                                                   0.086
                                                                          0.114
                                      0.140
                                                    0.245
random
                              0.500
                                             0.188
                                                            0.353
                                                                   0.500
                                                                          0.162
shuffledataset
                              0.500
                                     0.088
                                             0.000
                                                    0.000
                                                            0.000
                                                                   1.000
                                                                          0.162
                                     0.060
D032_DFLpred
                              0.493
                                             0.130
                                                    0.114
                                                            0.101
                                                                   0.906
                                                                          0.164
                                fpr
                                        inf
                                               mcc
                                                       mk
                                                              npv
                                                                             tnr
                                                                                  \
                                                                     ppv
D029 SPOT-Disorder2
                              0.320
                                     0.439
                                             0.343
                                                    0.268
                                                            0.929
                                                                   0.339
                                                                          0.680
D013 fIDPln
                              0.147
                                     0.359
                                             0.327
                                                    0.298
                                                            0.899
                                                                   0.399
                                                                          0.853
D014 fIDPnn
                              0.048
                                     0.252
                                             0.327
                                                    0.424
                                                            0.876
                                                                   0.548
                                                                          0.952
D025 RawMSA
                              0.279
                                      0.417
                                             0.323
                                                    0.251
                                                            0.925
                                                                   0.326
                                                                          0.721
D028 SPOT-Disorder1
                              0.334
                                     0.414
                                             0.311
                                                    0.234
                                                                   0.302
                                                            0.932
                                                                          0.666
D026_AUCpreD
                              0.296
                                     0.391
                                             0.303
                                                    0.235
                                                            0.919
                                                                   0.316 0.704
D002 Predisorder
                              0.417
                                      0.390
                                             0.292
                                                    0.219
                                                            0.937
                                                                   0.282
                                                                          0.583
D018_ESpritz-D
                              0.088
                                     0.264
                                             0.289
                                                    0.316
                                                            0.879
                                                                   0.437
                                                                          0.912
D008_IsUnstruct
                                     0.385
                                             0.287
                                                    0.214
                                                            0.929
                                                                   0.285
                              0.363
                                                                          0.637
D005_IUPred-long
                              0.280
                                     0.365
                                             0.285
                                                    0.222
                                                            0.913
                                                                   0.309
                                                                          0.720
D027_AUCpreD-np
                                                    0.233
                              0.226
                                     0.347
                                             0.284
                                                            0.904
                                                                   0.329
                                                                          0.774
```

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D003_IUPred2A-long
                             0.274
                                    0.360
                                           0.282
                                                  0.220
                                                         0.911
                                                                0.309
                                                                       0.726
                                           0.281
                                                  0.208
                                                                0.278
D021_MobiDB-lite
                             0.382
                                    0.379
                                                         0.930
                                                                       0.618
D030_SPOT-Disorder-Single
                             0.220
                                    0.337
                                           0.278
                                                  0.230
                                                         0.901
                                                                0.329
                                                                       0.780
D004_IUPred2A-short
                             0.225
                                    0.338
                                           0.278
                                                  0.229
                                                         0.902
                                                                0.327
                                                                       0.775
D024_DisoMine
                                    0.340
                                           0.277
                                                  0.225
                                                         0.903
                                                                0.322 0.765
                             0.235
D006_IUPred-short
                             0.227
                                    0.335
                                           0.275
                                                  0.225
                                                         0.901
                                                                0.324 0.773
D015 VSL2B
                             0.454 0.361
                                           0.266
                                                  0.196
                                                         0.939
                                                                0.257 0.546
D020_ESpritz-X
                             0.215
                                   0.317
                                           0.264
                                                  0.221
                                                         0.897
                                                                0.324 0.785
DO31 JRONN
                                           0.259
                                                  0.192
                                                                0.268 0.608
                             0.392 0.349
                                                         0.924
D019 ESpritz-N
                             0.347
                                   0.340
                                           0.256
                                                  0.192
                                                         0.915
                                                                0.277
                                                                       0.653
                             0.122 - 0.122
                                                  0.878
shuffletargets
                                           0.249
                                                         0.878
                                                                1.000 0.878
D011_DISOPRED-3.1
                             0.330
                                   0.317
                                           0.241
                                                  0.184
                                                         0.908
                                                                0.276 0.670
D001_PyHCA
                             0.341
                                    0.318
                                           0.240
                                                  0.181
                                                         0.909
                                                                0.272 0.659
new-pdb-r_simple
                             0.669
                                    0.262
                                           0.213
                                                  0.173
                                                         0.961
                                                                0.212 0.331
D007 FoldUnfold
                                   0.284
                                                                0.251 0.618
                             0.382
                                           0.211
                                                  0.157
                                                         0.906
D017_DisEMBL-465
                             0.164
                                   0.223
                                           0.206
                                                  0.189
                                                         0.876
                                                                0.313 0.836
                                                                0.242 0.680
D016_DisEMBL-HL
                             0.320
                                   0.210
                                           0.161
                                                  0.124
                                                         0.882
                                   0.177
                                                  0.123
                                                                0.252 0.761
D010_DisPredict-2
                             0.239
                                           0.147
                                                         0.871
D023_S2D-2
                             0.792 0.146
                                           0.138
                                                  0.131
                                                         0.945
                                                                0.186 0.208
D022_S2D-1
                             0.783
                                    0.142
                                                  0.123
                                                         0.937
                                                                0.186 0.217
                                           0.132
                                                  0.079
D009_GlobPlot
                             0.597
                                   0.138
                                           0.105
                                                         0.887
                                                                0.192 0.403
                                                                0.225 0.757
                             0.243 0.122
                                           0.102
                                                  0.085
                                                         0.860
D033 DynaMine
new-disprot-all_simple_cons
                             0.871 0.043
                                           0.049
                                                  0.055
                                                         0.886
                                                                0.169 0.129
                             0.501 -0.001
                                           0.000
                                                  0.000
                                                                0.162 0.499
random
                                                         0.838
shuffledataset
                             0.162 -0.162
                                           0.000
                                                  0.838
                                                         0.838
                                                                1.000
                                                                       0.838
D032 DFLpred
                             0.109 -0.015 -0.017 -0.020
                                                         0.836
                                                                0.144 0.891
                                    aucroc
                                            aucpr
                                                     aps
                                                            thr
                               tpr
D029_SPOT-Disorder2
                             0.759
                                     0.760
                                            0.340 0.340
                                                          0.370
                                            0.422
D013_fIDPln
                             0.506
                                     0.793
                                                   0.421
                                                          0.353
                                            0.475
                                                  0.475
D014_fIDPnn
                             0.300
                                     0.814
                                                          0.505
D025_RawMSA
                                     0.779
                                            0.386
                                                   0.385
                                                          0.500
                             0.696
                                            0.268
D028_SP0T-Disorder1
                             0.748
                                     0.744
                                                   0.268
                                                          0.460
D026_AUCpreD
                             0.687
                                     0.757
                                            0.479
                                                   0.312
                                                          0.500
D002_Predisorder
                             0.807
                                     0.747
                                            0.325 0.324
                                                          0.500
D018_ESpritz-D
                             0.352
                                     0.774
                                            0.410 0.409
                                                          0.508
D008 IsUnstruct
                             0.748
                                            0.323 0.314
                                                          0.500
                                     0.744
D005_IUPred-long
                             0.645
                                     0.737
                                            0.298 0.298
                                                          0.502
D027 AUCpreD-np
                             0.573
                                     0.751
                                            0.427
                                                   0.316
                                                          0.500
D003 IUPred2A-long
                                            0.298
                                                  0.298
                                                          0.502
                             0.634
                                     0.735
D021 MobiDB-lite
                             0.761
                                     0.737
                                            0.366 0.326
                                                          0.250
D030 SPOT-Disorder-Single
                             0.557
                                     0.757
                                            0.318 0.318
                                                          0.426
D004 IUPred2A-short
                                     0.741
                                            0.313 0.312
                                                          0.501
                             0.563
D024_DisoMine
                             0.575
                                     0.765
                                            0.388 0.388
                                                          0.376
D006_IUPred-short
                                     0.739
                             0.562
                                            0.311
                                                   0.311
                                                          0.501
D015_VSL2B
                             0.815
                                     0.732
                                            0.301
                                                   0.296
                                                          0.500
D020_ESpritz-X
                             0.532
                                     0.739
                                            0.304
                                                   0.303
                                                          0.144
```

DO31_JRONN	0.741	0.724	0.302	0.301	0.500
D019_ESpritz-N	0.687	0.714	0.296	0.296	0.309
shuffletargets	0.000	0.624	0.421	0.239	1.000
D011_DISOPRED-3.1	0.647	0.701	0.290	0.260	0.500
D001_PyHCA	0.659	0.706	0.277	0.277	0.500
new-pdb-r_simple	0.931	0.634	0.528	0.209	0.067
D007_FoldUnfold	0.666	0.642	0.485	0.221	1.000
D017_DisEMBL-465	0.387	0.685	0.283	0.282	0.500
D016_DisEMBL-HL	0.530	0.654	0.274	0.274	0.086
D010_DisPredict-2	0.416	0.637	0.250	0.250	0.500
D023_S2D-2	0.938	0.654	0.230	0.230	0.288
D022_S2D-1	0.925	0.672	0.253	0.253	0.335
D009_GlobPlot	0.735	0.616	0.242	0.240	0.290
D033_DynaMine	0.365	0.603	0.236	0.235	0.500
new-disprot-all_simple_cons	0.914	0.567	0.193	0.193	0.400
random	0.500	0.500	0.163	0.162	0.500
shuffledataset	0.000	0.500	0.230	0.162	1.000
D032_DFLpred	0.094	0.410	0.142	0.143	0.180

0.1.2 Metrics calculated at target level

	bac	csi	f05	f1s	f2s	fnr	fom	\
D029_SPOT-Disorder2	0.701	0.385	0.455	0.479	0.540	0.314	0.198	
D025_RawMSA	0.697	0.369	0.440	0.458	0.514	0.348	0.180	
D028_SPOT-Disorder1	0.681	0.361	0.437	0.450	0.501	0.353	0.196	
D026_AUCpreD	0.675	0.349	0.404	0.420	0.472	0.398	0.195	
D005_IUPred-long	0.659	0.312	0.398	0.403	0.445	0.436	0.182	
shuffletargets	0.624	0.227	0.000	0.000	0.000	1.000	0.122	
D003_IUPred2A-long	0.656	0.308	0.396	0.400	0.439	0.447	0.185	
D002_Predisorder	0.688	0.332	0.393	0.440	0.537	0.238	0.169	
D011_DISOPRED-3.1	0.644	0.298	0.389	0.385	0.418	0.460	0.198	
D004_IUPred2A-short	0.648	0.299	0.398	0.393	0.420	0.497	0.197	
D008_IsUnstruct	0.675	0.326	0.393	0.429	0.509	0.308	0.180	
D006_IUPred-short	0.647	0.297	0.397	0.392	0.419	0.497	0.197	
D027_AUCpreD-np	0.641	0.307	0.387	0.383	0.412	0.505	0.207	
DO31_JRONN	0.671	0.311	0.384	0.416	0.492	0.328	0.176	
D020_ESpritz-X	0.635	0.297	0.392	0.387	0.414	0.508	0.201	
D015_VSL2B	0.677	0.318	0.377	0.425	0.525	0.238	0.179	
D019_ESpritz-N	0.660	0.302	0.382	0.402	0.465	0.376	0.185	
D021_MobiDB-lite	0.673	0.320	0.399	0.421	0.480	0.384	0.174	
D013_fIDPln	0.647	0.331	0.408	0.416	0.460	0.452	0.236	
D030_SPOT-Disorder-Single	0.625	0.294	0.389	0.374	0.391	0.544	0.209	
D024_DisoMine	0.634	0.320	0.399	0.405	0.450	0.427	0.244	
D014_fIDPnn	0.619	0.289	0.394	0.360	0.360	0.617	0.252	
new-pdb-r_simple	0.668	0.342	0.382	0.440	0.563	0.101	0.346	
D001_PyHCA	0.641	0.290	0.366	0.390	0.455	0.390	0.196	

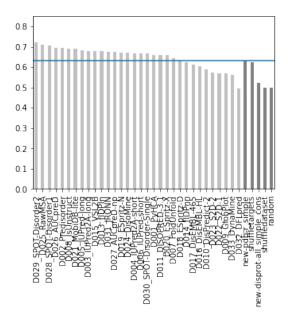
```
D018_ESpritz-D
                              0.617
                                     0.335
                                            0.428
                                                   0.414
                                                          0.438
                                                                  0.494 0.340
                                            0.234
                                                   0.259
D033_DynaMine
                              0.606
                                     0.179
                                                           0.335
                                                                  0.476
                                                                        0.152
D017_DisEMBL-465
                              0.588
                                     0.229
                                            0.351
                                                   0.326
                                                           0.329
                                                                  0.639
                                                                         0.223
                                                   0.000
D007_FoldUnfold
                              0.620
                                     0.286
                                            0.000
                                                           0.000
                                                                  1.000 0.408
D016_DisEMBL-HL
                              0.605
                                    0.241
                                            0.323
                                                   0.345
                                                           0.407
                                                                  0.451 0.212
D023_S2D-2
                              0.601
                                    0.269
                                            0.308
                                                   0.369
                                                           0.506
                                                                  0.079 0.164
                                     0.240
                                            0.310
                                                   0.345
                                                           0.438
                                                                  0.292 0.203
D009 GlobPlot
                              0.589
                                                                  0.093 0.191
D022 S2D-1
                              0.598
                                     0.266
                                            0.307
                                                   0.367
                                                           0.501
                                            0.290
                                                   0.343
                                                                  0.122 0.204
new-disprot-all simple cons
                              0.559
                                     0.247
                                                           0.469
D010 DisPredict-2
                              0.548
                                     0.213
                                            0.286
                                                   0.291
                                                           0.330
                                                                  0.566 0.258
D032 DFLpred
                                     0.080
                                                   0.126
                                                                  0.861
                              0.504
                                            0.142
                                                           0.126
                                                                         0.202
random
                              0.500
                                     0.140
                                            0.188
                                                   0.245
                                                           0.353
                                                                  0.500
                                                                         0.162
                                                           0.000
shuffledataset
                              0.500
                                    0.088
                                            0.000
                                                   0.000
                                                                  1.000
                                                                         0.162
                                fpr
                                       inf
                                              mcc
                                                      mk
                                                             npv
                                                                    ppv
                                                                           tnr
                                                                  0.459
D029_SPOT-Disorder2
                              0.301
                                     0.373
                                            0.305
                                                   0.261
                                                           0.802
                                                                         0.699
                              0.274
                                                   0.273
                                                                  0.453
D025_RawMSA
                                    0.363
                                            0.300
                                                           0.820
                                                                         0.726
D028_SP0T-Disorder1
                              0.302
                                     0.332
                                            0.282
                                                   0.256
                                                                  0.453
                                                           0.804
                                                                         0.698
D026_AUCpreD
                              0.283
                                    0.322
                                            0.270
                                                   0.243
                                                           0.805
                                                                  0.439
                                                                         0.717
D005_IUPred-long
                              0.260
                                    0.289
                                            0.250
                                                   0.262
                                                           0.818
                                                                  0.444
                                                                         0.740
                              0.122 -0.122
                                                   0.878
                                                                  1.000
shuffletargets
                                            0.249
                                                           0.878
                                                                         0.878
                                                                         0.747
D003 IUPred2A-long
                              0.253
                                     0.285
                                            0.247
                                                   0.258
                                                           0.815
                                                                  0.443
D002_Predisorder
                              0.412
                                    0.342
                                            0.247
                                                   0.206
                                                          0.831
                                                                  0.375
                                                                         0.588
                              0.253
                                    0.285
                                            0.245
                                                   0.256
                                                                  0.454
D011 DISOPRED-3.1
                                                           0.802
                                                                         0.747
D004 IUPred2A-short
                              0.210
                                     0.283
                                            0.242
                                                   0.229
                                                           0.803
                                                                  0.425
                                                                         0.790
D008 IsUnstruct
                              0.360
                                    0.322
                                            0.242
                                                   0.205
                                                           0.820
                                                                  0.386
                                                                         0.640
                                    0.281
D006 IUPred-short
                              0.211
                                            0.240
                                                   0.230
                                                          0.803
                                                                  0.427
                                                                         0.789
D027_AUCpreD-np
                              0.224 0.273
                                            0.239
                                                   0.228
                                                           0.793
                                                                  0.435
                                                                         0.776
DO31_JRONN
                              0.361
                                    0.304
                                            0.237
                                                   0.208
                                                           0.824
                                                                  0.384
                                                                         0.639
                              0.217
                                    0.266
                                            0.233
                                                   0.225
                                                                  0.426
D020_ESpritz-X
                                                          0.799
                                                                         0.783
D015_VSL2B
                              0.436
                                    0.320
                                            0.232
                                                   0.181
                                                                  0.360
                                                           0.821
                                                                         0.564
                                            0.232
                                                   0.203
                                                                  0.388
D019_ESpritz-N
                              0.313
                                    0.303
                                                          0.815
                                                                         0.687
                              0.392
                                    0.213
                                            0.231
                                                   0.227
                                                                  0.400
D021_MobiDB-lite
                                                           0.826
                                                                         0.608
                                                   0.214
D013_fIDPln
                              0.273
                                    0.248
                                            0.227
                                                          0.764
                                                                  0.449
                                                                         0.727
D030_SPOT-Disorder-Single
                              0.205
                                    0.235
                                            0.223
                                                   0.238
                                                          0.791
                                                                  0.447
                                                                         0.795
D024_DisoMine
                              0.326
                                    0.223
                                            0.209
                                                   0.191
                                                           0.756
                                                                  0.435
                                                                         0.674
D014 fIDPnn
                              0.151
                                    0.195
                                            0.205
                                                   0.283
                                                          0.748
                                                                  0.535
                                                                         0.849
new-pdb-r_simple
                              0.600
                                    0.295
                                            0.204
                                                   0.013
                                                          0.654
                                                                  0.359
                                                                         0.400
D001 PyHCA
                              0.341
                                    0.259
                                            0.199
                                                   0.177
                                                           0.804
                                                                  0.373
                                                                         0.659
D018 ESpritz-D
                              0.293
                                    0.177
                                            0.182
                                                   0.161
                                                           0.660
                                                                  0.501
                                                                         0.707
                              0.297
                                     0.241
                                                   0.174
                                                                  0.326
D033 DynaMine
                                            0.173
                                                          0.848
                                                                         0.703
D017_DisEMBL-465
                              0.170 0.181
                                            0.169
                                                   0.172
                                                           0.777
                                                                  0.395
                                                                         0.830
D007 FoldUnfold
                              0.382 -0.382
                                            0.169
                                                   0.592
                                                          0.592
                                                                  1.000 0.618
D016_DisEMBL-HL
                              0.350 0.191
                                            0.136
                                                   0.111
                                                          0.788
                                                                  0.323
                                                                         0.650
                              0.771
                                    0.149
                                                   0.119
                                                                  0.283
D023_S2D-2
                                            0.122
                                                          0.836
                                                                         0.229
D009_GlobPlot
                              0.549
                                     0.167
                                            0.121
                                                   0.100
                                                           0.797
                                                                  0.302
                                                                         0.451
D022_S2D-1
                              0.760
                                    0.146
                                            0.116
                                                   0.091
                                                           0.809
                                                                  0.283
                                                                        0.240
```

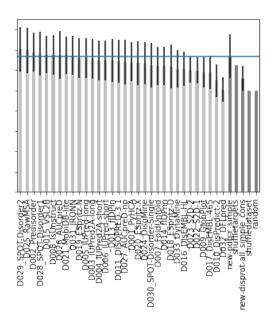
new-disprot-all_simple_cons	0.810	0.077	0.067	0.073	0.796	0.276	0.190
D010_DisPredict-2	0.352		0.055	0.064	0.742	0.322	0.648
D032_DFLpred	0.118		0.018	0.014	0.798	0.216	0.882
random		-0.001		0.000	0.838	0.162	
shuffledataset		-0.162		0.838		1.000	0.838
2	0.100	01202		0.000	0.000	_,,,,	0.000
	tpr	thr	aucroc	aucpr	aps		
D029_SPOT-Disorder2	0.686	0.370	NaN	NaN	NaN		
D025_RawMSA	0.652	0.500	NaN	NaN	NaN		
D028_SP0T-Disorder1	0.647	0.460	NaN	NaN	NaN		
D026_AUCpreD	0.602	0.500	NaN	NaN	NaN		
D005_IUPred-long	0.564	0.502	NaN	NaN	NaN		
shuffletargets	0.000	1.000	0.624	0.421	0.239		
D003_IUPred2A-long	0.553	0.502	NaN	NaN	NaN		
D002_Predisorder	0.762	0.500	NaN	NaN	NaN		
D011_DISOPRED-3.1	0.540	0.500	NaN	NaN	NaN		
D004_IUPred2A-short	0.503	0.501	NaN	NaN	NaN		
D008_IsUnstruct	0.692	0.500	NaN	NaN	NaN		
D006_IUPred-short	0.503	0.501	NaN	NaN	NaN		
D027_AUCpreD-np	0.495	0.500	NaN	NaN	NaN		
DO31_JRONN	0.672	0.500	NaN	NaN	NaN		
D020_ESpritz-X	0.492	0.144	NaN	NaN	NaN		
D015_VSL2B	0.762	0.500	NaN	NaN	NaN		
D019_ESpritz-N	0.624	0.309	NaN	NaN	NaN		
DO21_MobiDB-lite	0.616	0.250	NaN	NaN	NaN		
D013_fIDPln	0.548	0.353	NaN	NaN	NaN		
D030_SPOT-Disorder-Single	0.456	0.426	NaN	NaN	NaN		
D024_DisoMine	0.573	0.376	NaN	NaN	NaN		
D014_fIDPnn	0.383	0.505	NaN	NaN	NaN		
new-pdb-r_simple	0.899	0.067	NaN	NaN	NaN		
DO01_PyHCA	0.610	0.500	NaN	NaN	NaN		
D018_ESpritz-D	0.506	0.508	NaN	NaN	NaN		
D033_DynaMine	0.524	0.500	NaN	NaN	NaN		
D017_DisEMBL-465	0.361	0.500	NaN	NaN	NaN		
D007_FoldUnfold	0.000	1.000	NaN	NaN	NaN		
D016_DisEMBL-HL	0.549	0.086	NaN	NaN	NaN		
D023_S2D-2	0.921	0.288	NaN	NaN	NaN		
D009_GlobPlot	0.708	0.290	NaN	NaN	NaN		
D022_S2D-1	0.907	0.335	NaN	NaN	NaN		
new-disprot-all_simple_cons	0.878	0.400	NaN	NaN	NaN		
D010_DisPredict-2	0.434	0.500	NaN	NaN	NaN		
D032_DFLpred	0.139	0.180	NaN	NaN	NaN		
random	0.500	0.500	0.500	0.163	0.162		
shuffledataset	0.000	1.000	0.500	0.230	0.162		

0.2 Plot of single metrics at dataset and target levels with errors

0.2.1 Balanced accuracy

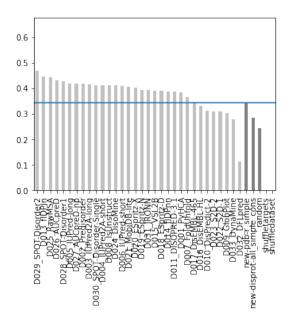
- dataset level (sx); error: confidence interval calculated on 1000-rounds bootstrap (invisible since too small)
- target level (dx); standard deviation

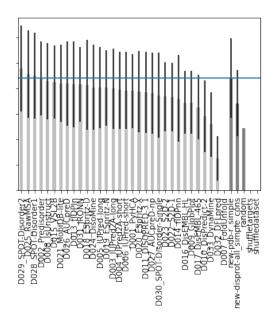




0.2.2 F 1 score

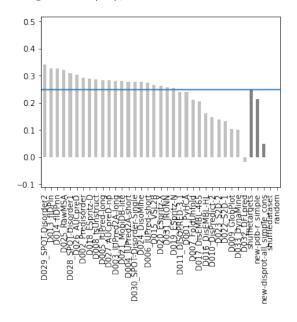
- dataset level (sx); error: confidence interval calculated on 1000-rounds bootstrap (invisible since too small)
- target level (dx); standard deviation

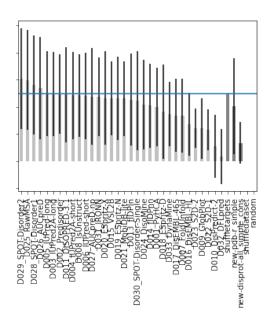




0.2.3 MCC

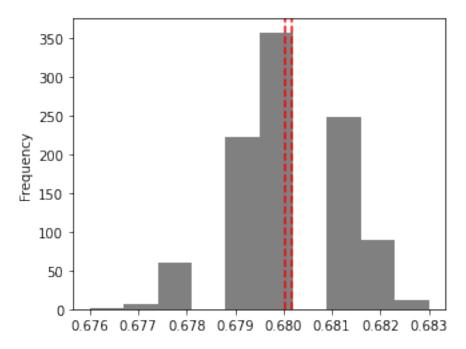
- \bullet dataset level (sx); error: confidence interval calculated on 1000-rounds bootstrap (invisible since too small)
- target level (dx); standard deviation





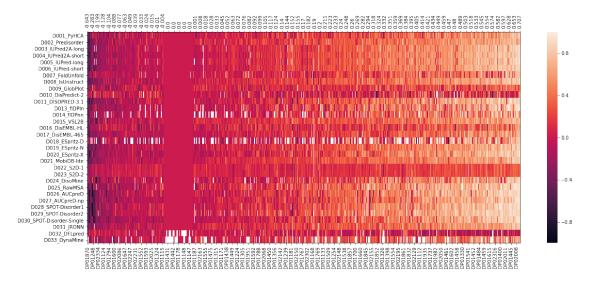
0.3 Example of confidence interval

Confidence Interval for the distribution of 1000 Balanced Accuracy (calculated at the dataset level) scores for IUpred2A.



0.4 MCC per target per predictor

Heatmap representing the MCC for each target for each predictor. Sorted by average-target MCC (big-->small), which can be seen on upper tick labels.

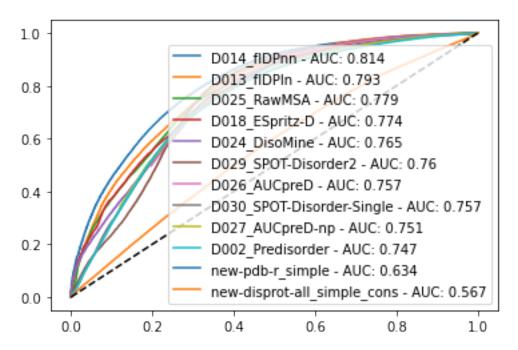


0.5 Predictor correlation

MCC calculated at the target level of all predictors against all predictors. Each point is a target, their coordinates are their MCC calculated from predictor x and predictor y. The Diagonal shows the distribution of MCC for predictor x=y

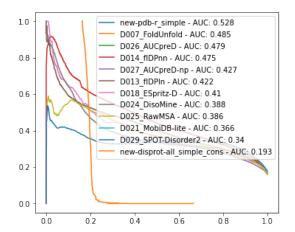
0.5.1 ROC curve

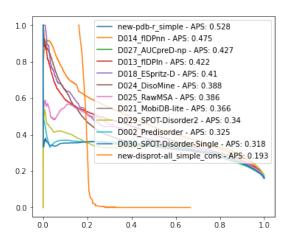
ROC curve. x axis 1-specificity; y axis sensitivity. Only first 10 best ranking methods are shown. Ranking is based on ROC AUC.



0.5.2 Precision-Recall curve

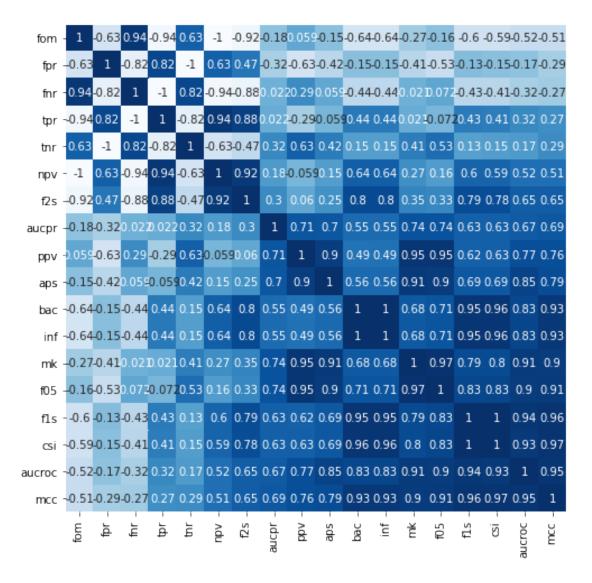
Precision-Recall curve. x axis recall; y axis precision. Only first 10 best ranking methods are shown. * (sx) Ranking is based on PR AUC * (dx) Ranking is based on APS (average precision score)





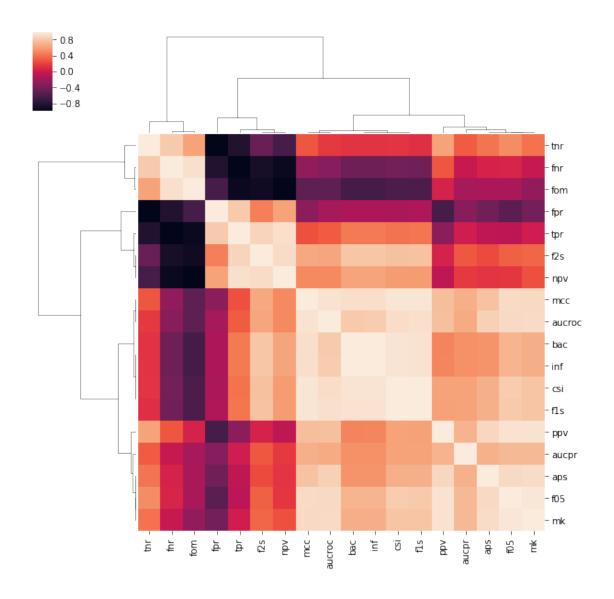
0.6 Metrics correlation

0.6.1 Pearson correlation between metrics calculated at the dataset level



0.6.2 Clustering between metrics calculated at the dataset level

Clustering distance is calculated as correlation



0.7 Ranking

0.7.1 Raw ranking of each metric

	bac	csi	f05	f1s	f2s	fnr	fom	fpr	\
D029_SP0T-Disorder2	1.0	1.0	4.0	1.0	1.0	30.0	30.0	18.0	
D025_RawMSA	2.0	3.0	5.0	3.0	5.0	25.0	28.0	21.0	
D013_fIDPln	11.0	2.0	3.0	2.0	25.0	10.0	14.0	33.0	
D026_AUCpreD	4.0	4.0	10.0	4.0	8.0	24.0	26.0	19.0	
D027_AUCpreD-np	13.0	6.0	6.0	8.0	19.0	16.0	19.0	27.0	
D002_Predisorder	5.0	8.0	18.0	8.0	2.0	32.0	34.0	8.0	
D028_SP0T-Disorder1	3.0	5.0	15.0	5.0	3.0	29.0	32.0	15.0	

```
D014_fIDPnn
                               25.0
                                     21.0
                                             1.0
                                                  21.0
                                                         33.0
                                                                 4.0
                                                                       7.0
                                                                             37.0
                                                   13.0
                                                          7.0
                                                                29.0
                                                                             12.0
D008 IsUnstruct
                                6.0
                                     13.0
                                            17.0
                                                                      30.0
D024_DisoMine
                               15.0
                                      13.0
                                            11.0
                                                   13.0
                                                         20.0
                                                                17.0
                                                                      18.0
                                                                             25.0
                                             3.0
                                                         31.0
                                                                 5.0
D018_ESpritz-D
                               23.0
                                      20.0
                                                   20.0
                                                                       9.0
                                                                             36.0
D030_SPOT-Disorder-Single
                               18.0
                                     11.0
                                             7.0
                                                   11.0
                                                         23.0
                                                                13.0
                                                                      16.0
                                                                             29.0
D005_IUPred-long
                                8.0
                                       8.0
                                            13.0
                                                    8.0
                                                         12.0
                                                                19.0
                                                                      24.0
                                                                             20.0
D021 MobiDB-lite
                                7.0
                                     15.0
                                            19.0
                                                   15.0
                                                          7.0
                                                                31.0
                                                                      31.0
                                                                             11.0
                                                   11.0
                                                         21.0
D004_IUPred2A-short
                               16.0
                                      11.0
                                             8.0
                                                                15.0
                                                                      17.0
                                                                             28.0
D003 IUPred2A-long
                                            14.0
                                                    9.0
                                                         13.0
                                                                18.0
                                                                      23.0
                                                                             22.0
                               10.0
                                       9.0
D006 IUPred-short
                               18.0
                                      14.0
                                            10.0
                                                   14.0
                                                         22.0
                                                                14.0
                                                                      16.0
                                                                             26.0
D020 ESpritz-X
                               21.0
                                      16.0
                                            12.0
                                                   16.0
                                                         26.0
                                                                12.0
                                                                      13.0
                                                                             30.0
D015_VSL2B
                               10.0
                                      19.0
                                            24.0
                                                   19.0
                                                          4.0
                                                                33.0
                                                                      35.0
                                                                              7.0
DO31 JRONN
                               12.0
                                      18.0
                                            23.0
                                                   18.0
                                                         10.0
                                                                27.0
                                                                      27.0
                                                                              9.0
D019_ESpritz-N
                               15.0
                                     17.0
                                            20.0
                                                   17.0
                                                         12.0
                                                                24.0
                                                                      25.0
                                                                             13.0
                                     22.0
                                            21.0
                                                   22.0
                                                         17.0
                                                                20.0
                                                                      21.0
                                                                             16.0
D011_DISOPRED-3.1
                               20.0
D001_PyHCA
                               20.0
                                     23.0
                                            22.0
                                                   23.0
                                                         16.0
                                                                21.0
                                                                      22.0
                                                                             14.0
                                      25.0
                                            25.0
                                                   24.0
                                                                      20.0
D007_FoldUnfold
                               22.0
                                                         18.0
                                                                22.0
                                                                             11.0
new-pdb-r_simple
                               24.0
                                      27.0
                                            28.0
                                                   26.0
                                                          9.0
                                                                36.0
                                                                      37.0
                                                                              4.0
                                                   25.0
                                                         29.0
                                                                 7.0
                                                                       7.0
D017_DisEMBL-465
                               27.0
                                      26.0
                                            17.0
                                                                             31.0
shuffletargets
                               26.0
                                      24.0
                                            37.0
                                                   37.0
                                                         37.0
                                                                 2.0
                                                                       8.0
                                                                             34.0
D016_DisEMBL-HL
                               28.0
                                      28.0
                                            27.0
                                                   27.0
                                                         28.0
                                                                11.0
                                                                      10.0
                                                                             18.0
D010 DisPredict-2
                               29.0
                                     29.0
                                            26.0
                                                   28.0
                                                         30.0
                                                                 8.0
                                                                       5.0
                                                                             24.0
D022_S2D-1
                               31.0
                                     31.0
                                            32.0
                                                   30.0
                                                         15.0
                                                                35.0
                                                                      34.0
                                                                              3.0
D023 S2D-2
                               30.0
                                      30.0
                                            31.0
                                                   30.0
                                                         14.0
                                                                37.0
                                                                      36.0
                                                                              2.0
shuffledataset
                               36.0
                                      36.0
                                            37.0
                                                   37.0
                                                         37.0
                                                                 2.0
                                                                       3.0
                                                                             32.0
D009 GlobPlot
                               32.0
                                      32.0
                                            30.0
                                                   31.0
                                                         27.0
                                                                26.0
                                                                      12.0
                                                                              5.0
D033 DynaMine
                                                                 6.0
                               33.0
                                      34.0
                                            29.0
                                                   33.0
                                                         34.0
                                                                       4.0
                                                                             23.0
new-disprot-all simple cons
                               34.0
                                      33.0
                                            33.0
                                                   32.0
                                                         24.0
                                                                34.0
                                                                      11.0
                                                                              1.0
random
                               36.0
                                      35.0
                                            34.0
                                                   34.0
                                                         32.0
                                                                 9.0
                                                                       3.0
                                                                              6.0
D032_DFLpred
                               37.0
                                      37.0
                                            35.0
                                                   35.0
                                                         35.0
                                                                 3.0
                                                                             35.0
                                                                       1.0
                                                    npv
                                                                             aucroc
                                inf
                                       mcc
                                              mk
                                                          ppv
                                                                 tnr
                                                                       tpr
D029_SPOT-Disorder2
                                1.0
                                             6.0
                                                    9.0
                                                          6.0
                                                                21.0
                                                                       8.0
                                                                                6.0
                                       1.0
                                2.0
                                                                17.0
                                                                      13.0
D025_RawMSA
                                       4.0
                                             7.0
                                                   10.0
                                                         10.0
                                                                                3.0
D013_fIDPln
                               11.0
                                       3.0
                                             5.0
                                                   24.0
                                                          5.0
                                                                 5.0
                                                                      28.0
                                                                                2.0
D026_AUCpreD
                                4.0
                                       6.0
                                             8.0
                                                   12.0
                                                         14.0
                                                                19.0
                                                                      15.0
                                                                                8.0
D027 AUCpreD-np
                               13.0
                                      11.0
                                            10.0
                                                   19.0
                                                          8.0
                                                                11.0
                                                                      22.0
                                                                                9.0
D002 Predisorder
                                5.0
                                       7.0
                                            18.0
                                                    5.0
                                                         20.0
                                                                30.0
                                                                       6.0
                                                                               10.0
D028 SPOT-Disorder1
                                3.0
                                       5.0
                                             9.0
                                                    6.0
                                                         18.0
                                                                23.0
                                                                      10.0
                                                                               12.0
D014 fIDPnn
                               25.0
                                       3.0
                                             3.0
                                                   32.0
                                                          3.0
                                                                 1.0
                                                                      34.0
                                                                                1.0
D008 IsUnstruct
                                6.0
                                            19.0
                                                    9.0
                                                         19.0
                                                                26.0
                                                                      10.0
                                                                               12.0
                                       9.0
D024_DisoMine
                               15.0
                                      16.0
                                            14.0
                                                   20.0
                                                         13.0
                                                                13.0
                                                                      21.0
                                                                                5.0
D018 ESpritz-D
                               23.0
                                       8.0
                                             4.0
                                                   29.0
                                                          4.0
                                                                 2.0
                                                                      33.0
                                                                                4.0
                                                   23.0
D030_SPOT-Disorder-Single
                               17.0
                                     15.0
                                            11.0
                                                          8.0
                                                                 9.0
                                                                      25.0
                                                                                8.0
D005_IUPred-long
                                      10.0
                                            15.0
                                                   14.0
                                                         17.0
                                                                18.0
                                                                               17.0
                                8.0
                                                                      19.0
                                                    7.0
D021_MobiDB-lite
                                7.0
                                      13.0
                                            20.0
                                                         21.0
                                                                28.0
                                                                       7.0
                                                                               17.0
                                                   21.0
                                                          9.0
D004_IUPred2A-short
                               16.0
                                      15.0
                                            12.0
                                                                10.0
                                                                      23.0
                                                                               13.0
```

D003_IUPred2A-long	10.0	12.0	17.0	15.0	17.0	16.0	20.0	18.0
D006_IUPred-short	18.0	17.0	14.0	23.0	12.0	12.0	24.0	15.0
D020_ESpritz-X	21.0	19.0	16.0	25.0	12.0	8.0	26.0	15.0
D015_VSL2B	9.0	18.0	21.0	3.0	26.0	31.0	5.0	19.0
DO31_JRONN	12.0	20.0	23.0	11.0	25.0	29.0	11.0	20.0
D019_ESpritz-N	15.0	21.0	23.0	13.0	22.0	25.0	15.0	21.0
D011_DISOPRED-3.1	21.0	23.0	25.0	17.0	23.0	22.0	18.0	23.0
D001_PyHCA	19.0	24.0	26.0	16.0	24.0	24.0	17.0	22.0
D007_FoldUnfold	22.0	26.0	28.0	18.0	28.0	28.0	16.0	28.0
new-pdb-r_simple	24.0	25.0	27.0	1.0	31.0	34.0	2.0	30.0
D017_DisEMBL-465	26.0	27.0	24.0	32.0	15.0	7.0	31.0	24.0
shuffletargets	36.0	22.0	1.0	30.0	2.0	4.0	37.0	31.0
D016_DisEMBL-HL	27.0	28.0	30.0	28.0	29.0	21.0	27.0	27.0
D010_DisPredict-2	28.0	29.0	32.0	33.0	27.0	14.0	30.0	29.0
D022_S2D-1	30.0	31.0	32.0	5.0	34.0	35.0	3.0	25.0
D023_S2D-2	29.0	30.0	29.0	2.0	34.0	36.0	1.0	27.0
shuffledataset	37.0	36.0	2.0	36.0	2.0	6.0	37.0	36.0
D009_GlobPlot	31.0	32.0	34.0	26.0	32.0	33.0	12.0	32.0
D033_DynaMine	32.0	33.0	33.0	34.0	30.0	15.0	32.0	33.0
new-disprot-all_simple_cons	33.0	34.0	35.0	27.0	35.0	37.0	4.0	34.0
random	34.0	36.0	36.0	36.0	36.0	32.0	29.0	36.0
D032_DFLpred	35.0	37.0	37.0	37.0	37.0	3.0	35.0	37.0
	aucpr	aps						
D029_SPOT-Disorder2	12.0	6.0						
D025_RawMSA	10.0	5.0						
D013_fIDPln	6.0	2.0						
D026_AUCpreD	3.0	13.0						
D027_AUCpreD-np	5.0	10.0						
D002_Predisorder	13.0	8.0						
D028_SPOT-Disorder1	28.0	24.0						
D014_fIDPnn	4.0	1.0						
D008_IsUnstruct	14.0	11.0						
D024_DisoMine	9.0	4.0						
D018_ESpritz-D	8.0	3.0						
D030_SPOT-Disorder-Single	15.0	9.0						
D005_IUPred-long	22.0	18.0						
D021_MobiDB-lite	11.0	7.0						
D004_IUPred2A-short	16.0	13.0						
D003_IUPred2A-long	22.0	18.0						
D006_IUPred-short	17.0	14.0						
D020_ESpritz-X	18.0	15.0						
D015_VSL2B	20.0	20.0						
DO21 IDOMN	10 0	16 0						

19.0 16.0

23.0 20.0 24.0 25.0

26.0 22.0

DO31_JRONN

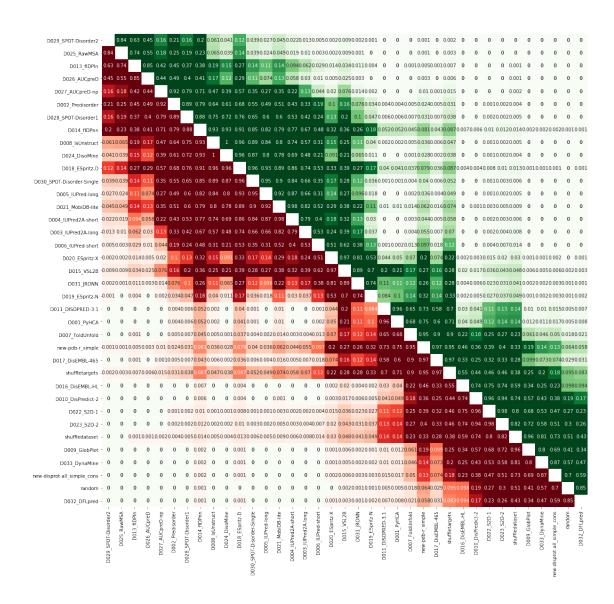
DO01_PyHCA

D019_ESpritz-N D011_DISOPRED-3.1

D007_FoldUnfold	2.0	32.0
new-pdb-r_simple	1.0	33.0
D017_DisEMBL-465	25.0	21.0
shuffletargets	7.0	29.0
D016_DisEMBL-HL	27.0	23.0
D010_DisPredict-2	30.0	27.0
D022_S2D-1	29.0	26.0
D023_S2D-2	34.0	31.0
shuffledataset	34.0	36.0
D009_GlobPlot	31.0	28.0
D033_DynaMine	32.0	30.0
new-disprot-all_simple_cons	35.0	34.0
random	36.0	36.0
D032_DFLpred	37.0	37.0

0.7.2 Average Overall Ranking

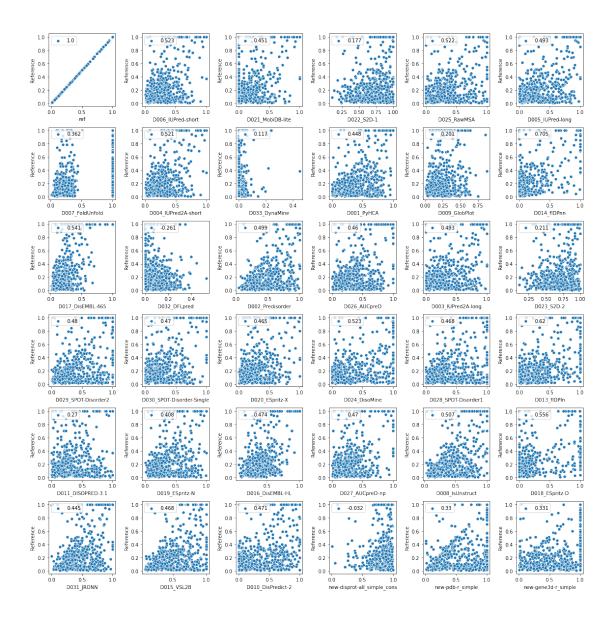
Average Overall ranking of predictors based on multiple metrics. For each metric a ranking is calculated so that each predictor has a distribution of rankings. The matrix represents the statistical significance (expressed as p-value) of the difference between distribution of rankings. The order of predictors in the matrix reflects the overall ranking (average of the distribution of ranking).



0.3541292880258076

0.8 Disorder content

Correlation between disorder content in the reference and predicted disorder content. Each dot is a protein in the dataset. The legend show Pearson R value.



0.9 Fully disordered

Performance of predictors on discriminate fully disordered proteins (>95% id content) from those

	tn	ÍР	in	tp
ref	529	0	0	40
D016_DisEMBL-HL	529	0	36	4
D032_DFLpred	529	0	40	0
D009_GlobPlot	529	0	40	0
D033_DynaMine	529	0	40	0
D017_DisEMBL-465	529	0	38	2
D006_IUPred-short	528	1	30	10

D004_IUPred2A-short	527	2	30	10
D021_MobiDB-lite	527	2	29	11
D019_ESpritz-N	525	4	28	12
D001_PyHCA	524	5	28	12
D011_DISOPRED-3.1	524	5	34	6
D020_ESpritz-X	523	6	31	9
D005_IUPred-long	523	6	25	15
D003_IUPred2A-long	523	6	27	13
DO31_JRONN	523	6	28	12
D030_SPOT-Disorder-Single	522	7	25	15
D027_AUCpreD-np	519	10	30	10
D026_AUCpreD	517	12	23	17
D002_Predisorder	517	12	21	19
D008_IsUnstruct	516	13	24	16
D014_fIDPnn	514	15	14	26
D010_DisPredict-2	514	15	27	13
D025_RawMSA	511	18	14	26
D015_VSL2B	506	23	17	23
D029_SPOT-Disorder2	503	26	19	21
D023_S2D-2	500	29	26	14
D028_SPOT-Disorder1	500	29	18	22
D013_fIDPln	498	31	14	26
D018_ESpritz-D	487	42	19	21
D024_DisoMine	481	48	13	27
D022_S2D-1	477	52	25	15
new-pdb-r_simple	412	117	8	32
new-gene3d-r_simple	394	135	3	37
new-disprot-all_simple_cons	393	136	34	6
D007_FoldUnfold	386	143	9	31