

A deep-learning approach toward rational molecular docking protocol selection.

Supplementary information

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Table 1: Predictive performance for RMSD_{\min} (± 1 std.) per docking protocol, for each of the four splits considered.

Protocol	RMSE	Pearson's R	RMSE	Pearson's R	RMSE	Pearson's R	RMSE	Pearson's R
	random		ligand scaffold		protein classes		protein classes balanced	
autodock-ga	1.74 (± 0.06)	0.51 (± 0.03)	1.85 (± 0.24)	0.35 (± 0.03)	1.81 (± 0.18)	0.44 (± 0.06)	1.64 (± 0.04)	0.59 (± 0.03)
autodock-lga	2.05 (± 0.06)	0.45 (± 0.04)	2.05 (± 0.43)	0.25 (± 0.14)	2.17 (± 0.13)	0.35 (± 0.07)	1.92 (± 0.05)	0.54 (± 0.04)
autodock-ls	2.37 (± 0.07)	0.27 (± 0.03)	2.22 (± 0.16)	0.20 (± 0.19)	2.24 (± 0.13)	0.37 (± 0.05)	2.29 (± 0.03)	0.37 (± 0.03)
glide-sp	2.32 (± 0.08)	0.42 (± 0.01)	2.34 (± 0.69)	0.23 (± 0.13)	2.34 (± 0.17)	0.37 (± 0.06)	2.06 (± 0.18)	0.52 (± 0.06)
gold-asp	1.97 (± 0.15)	0.45 (± 0.05)	1.82 (± 0.94)	0.21 (± 0.12)	1.99 (± 0.14)	0.45 (± 0.06)	1.81 (± 0.10)	0.59 (± 0.04)
gold-chemscore	2.35 (± 0.12)	0.40 (± 0.05)	2.18 (± 0.89)	0.20 (± 0.14)	2.27 (± 0.14)	0.46 (± 0.08)	2.12 (± 0.12)	0.56 (± 0.04)
gold-goldscore	1.98 (± 0.15)	0.32 (± 0.04)	1.70 (± 0.70)	-0.04 (± 0.48)	1.94 (± 0.21)	0.35 (± 0.09)	1.74 (± 0.11)	0.59 (± 0.21)
gold-plp	2.03 (± 0.18)	0.47 (± 0.06)	1.89 (± 0.96)	0.22 (± 0.15)	2.05 (± 0.20)	0.45 (± 0.08)	1.89 (± 0.04)	0.58 (± 0.02)
plants-chemplp	1.78 (± 0.17)	0.41 (± 0.05)	1.58 (± 0.72)	0.36 (± 0.34)	1.72 (± 0.23)	0.45 (± 0.03)	1.54 (± 0.12)	0.55 (± 0.04)
plants-plp95	2.35 (± 0.11)	0.41 (± 0.03)	2.14 (± 1.08)	0.12 (± 0.07)	2.34 (± 0.30)	0.38 (± 0.05)	2.01 (± 0.26)	0.52 (± 0.05)
plants-plp	2.18 (± 0.12)	0.39 (± 0.03)	1.90 (± 0.93)	0.15 (± 0.08)	2.06 (± 0.21)	0.45 (± 0.02)	1.87 (± 0.10)	0.50 (± 0.03)
rdock-solv	4.34 (± 0.25)	0.36 (± 0.05)	4.54 (± 0.51)	0.13 (± 0.09)	4.16 (± 0.52)	0.38 (± 0.08)	3.61 (± 0.26)	0.55 (± 0.02)
rdock-std	4.28 (± 0.10)	0.36 (± 0.03)	4.42 (± 0.65)	0.12 (± 0.08)	4.06 (± 0.49)	0.40 (± 0.08)	3.54 (± 0.18)	0.56 (± 0.01)
vina-std	2.08 (± 0.12)	0.27 (± 0.04)	2.40 (± 0.27)	0.05 (± 0.08)	2.11 (± 0.15)	0.28 (± 0.11)	1.92 (± 0.05)	0.37 (± 0.03)
Average	2.41 (± 0.12)	0.39 (± 0.04)	2.36 (± 0.66)	0.18 (± 0.15)	2.38 (± 0.23)	0.40 (± 0.07)	2.14 (± 0.12)	0.53 (± 0.05)

Table 2: Predictive performance for nRMSD (± 1 std.) per docking protocol, for each of the four splits considered.

Protocol	RMSE	Pearson's R	RMSE	Pearson's R	RMSE	Pearson's R	RMSE	Pearson's R
	random		ligand scaffold		protein classes		protein classes balanced	
autodock-ga	5.06 (± 0.43)	0.53 (± 0.04)	4.74 (± 1.54)	0.45 (± 0.3)	5.18 (± 0.21)	0.48 (± 0.06)	4.75 (± 0.2)	0.63 (± 0.03)
autodock-lga	6.87 (± 0.26)	0.52 (± 0.03)	5.62 (± 2.92)	0.23 (± 0.15)	7.23 (± 0.37)	0.45 (± 0.04)	6.65 (± 0.35)	0.59 (± 0.04)
autodock-ls	3.43 (± 0.27)	0.15 (± 0.13)	2.85 (± 0.92)	0.26 (± 0.37)	3.32 (± 0.35)	0.25 (± 0.14)	3.21 (± 0.15)	0.29 (± 0.06)
glide-sp	4.16 (± 0.1)	0.43 (± 0.02)	5.02 (± 1.39)	0.22 (± 0.14)	4.29 (± 0.38)	0.41 (± 0.07)	3.49 (± 0.16)	0.58 (± 0.03)
gold-asp	6.85 (± 0.11)	0.56 (± 0.02)	7.72 (± 0.39)	0.3 (± 0.17)	7.03 (± 0.47)	0.52 (± 0.06)	5.95 (± 0.09)	0.68 (± 0.01)
gold-chemscore	6.78 (± 0.1)	0.54 (± 0.02)	7.48 (± 0.89)	0.28 (± 0.15)	7.04 (± 0.37)	0.49 (± 0.03)	5.86 (± 0.13)	0.67 (± 0.02)
gold-goldscore	7.45 (± 0.19)	0.53 (± 0.02)	8.81 (± 0.77)	0.39 (± 0.31)	7.57 (± 0.33)	0.5 (± 0.05)	6.39 (± 0.2)	0.66 (± 0.02)
gold-plp	6.78 (± 0.09)	0.57 (± 0.01)	7.12 (± 0.9)	0.32 (± 0.18)	7.02 (± 0.51)	0.52 (± 0.06)	5.78 (± 0.17)	0.7 (± 0.02)
plants-chemplp	5.5 (± 0.12)	0.48 (± 0.01)	5.39 (± 1.75)	0.15 (± 0.09)	5.44 (± 0.31)	0.48 (± 0.06)	4.84 (± 0.09)	0.63 (± 0.02)
plants-plp95	4.91 (± 0.09)	0.48 (± 0.02)	6.03 (± 0.29)	0.09 (± 0.1)	5.08 (± 0.14)	0.47 (± 0.06)	4.39 (± 0.09)	0.63 (± 0.02)
plants-plp	5.07 (± 0.15)	0.47 (± 0.02)	6.05 (± 0.6)	0.12 (± 0.09)	5.11 (± 0.22)	0.48 (± 0.06)	4.52 (± 0.08)	0.63 (± 0.01)
rdock-solv	4.94 (± 0.17)	0.42 (± 0.03)	4.95 (± 0.93)	0.17 (± 0.09)	4.76 (± 0.33)	0.45 (± 0.07)	4.36 (± 0.23)	0.59 (± 0.02)
rdock-std	4.81 (± 0.15)	0.43 (± 0.03)	4.36 (± 1.57)	0.17 (± 0.09)	4.71 (± 0.38)	0.44 (± 0.08)	4.33 (± 0.19)	0.59 (± 0.03)
vina-std	0.94 (± 0.04)	0.1 (± 0.04)	0.89 (± 0.08)	0.64 (± 0.44)	0.94 (± 0.07)	0.15 (± 0.01)	0.9 (± 0.06)	0.31 (± 0.35)
Average	5.25 (± 0.16)	0.44 (± 0.03)	5.5 (± 1.07)	0.27 (± 0.19)	5.34 (± 0.32)	0.44 (± 0.06)	4.67 (± 0.16)	0.58 (± 0.05)

Table 3: Ligand-centric evaluation for the RMSD_{\min} (± 1 std.) metric and the four different proposed split types in this study.

Split type	Pearson's R	RMSE
random	0.45 (± 0.01)	2.20 (± 0.06)
ligand scaffold	0.49 (± 0.2)	2.19 (± 0.63)
protein classes	0.48 (± 0.03)	2.03 (± 0.19)
protein classes balanced	0.54 (± 0.01)	1.82 (± 0.07)

Table 4: Ligand-centric evaluation for the n RMSD(± 1 std.) metric and the four different proposed split types in this study.

Split type	Pearson's R	RMSE
random	0.55 (± 0.01)	4.88 (± 0.09)
ligand scaffold	0.57 (± 0.15)	5.77 (± 0.6)
protein classes	0.57 (± 0.04)	4.74 (± 0.26)
protein classes balanced	0.62 (± 0.01)	4.09 (± 0.06)

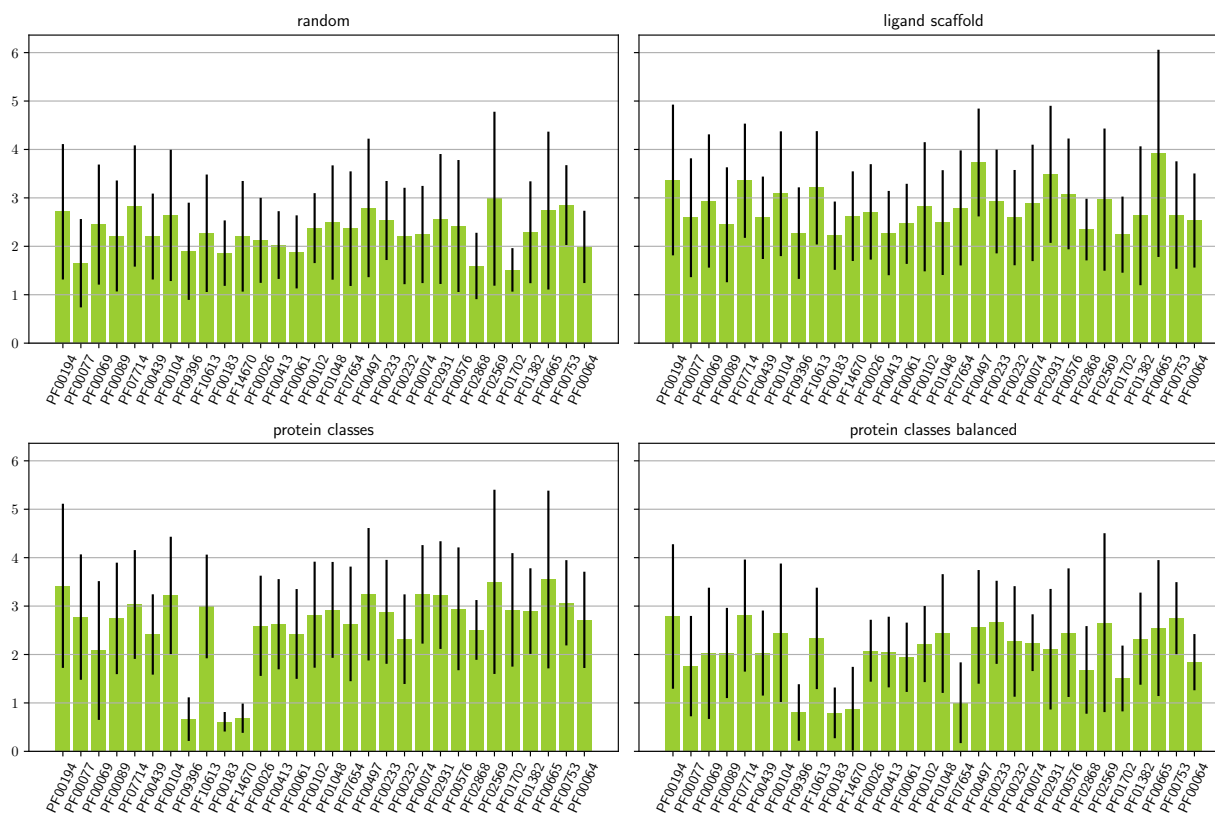


Figure 1: Average RMSE for the RMSD_{ave} metric for all types of splits disaggregated into the 30 most populated PFAM families in the PDBbind refined dataset.