DeeplyTough: Learning Structural Comparison of Protein Binding Sites

(Supporting Information)

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Figure S1: Box plots of TM-scores indicating the structurally similarity of pockets in a test set to their nearest neighbor pockets in a training set (again, in terms of TM-score) for each training scenario in this work. For TOUGH-M1 dataset, a single random permutation out of ten is visualized. The scores are computed with TM-align, with 1.0 indicating identity and 0.0 no alignment. Whiskers mark 1% and 99% percentiles of a distribution. Pockets in TOUGH-M1 can be defined in two ways: i) computationally with Fpocket 2.0 as used for training DeeplyTough (blue plots; top), or ii) around their bound ligands as in Vertex and ProSPECCTs (green plots; bottom). In general, the distributions suggest that there is no strong contamination between training and test sets (especially with computationally defined pockets), with only several pocket pairs being near-identical.
Figure S2: Precision-recall plot with associated average precision (AP) values evaluating the performance of pocket matching algorithms on TOUGH-M1 testing folds. Standard error, denoted as se, is measured over ten random splits.

Figure S3: Precision-recall plot with associated average precision (AP) values evaluating the performance of pocket matching algorithms on the Vertex dataset (6,977 protein pairs).
Table S1: AP values for DeeplyTough on each of ten ProSPECCTs datasets.

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<th>P2</th>
<th>P3</th>
<th>P4</th>
<th>P5</th>
<th>P5.2</th>
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References
