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We further investigated how the RMSD of ligand and the Tversky similarity of interaction fingerprints relate to the statistics of protein-ligand interaction. We visualized the results in Fig 8. We chose random structures from the subset of the 196 PDB files within TIP database and performed 100 docking runs. We calculated the average value of RMSD of ligand and the average value of Tversky similarity of interaction fingerprints for each of the random structures from the subset of the 196 PDB files as well as for the two reference structures. The sequences of the ligands were randomized as well. The red lines indicate the average RMSD values for the interactions with Glide XP and the blue lines indicate the average Tversky similarity of interaction fingerprints for the interactions with Mango-III. As we see, there is a clear correlation between RMSD of ligand and Tversky similarity of interaction fingerprints (R2 for linear least-squares regression equal 0.73; see Fig 8B and S15 Table). Note that the reference structures are excluded from the analysis due to the absence of any interactions. The correlation was also weak when the reference structures were included in the analysis (see S16 and S17 Tables). These results were similar when we calculated the RMSD of ligand or the Tversky similarity of interaction fingerprints independently (see Fig 8C and 8D). To further validate our method, we analyzed the combination of Glide XP and Mango-III with the DrugScore function of the BindN tool [81] of the DrugBank database [82] as a measure of binding affinity of the ligands. Note that it is known that the amino acid sequence of the binding pocket in a protein is the single most important factor that determines the binding affinity of a ligand to that binding site [83, 84]. Among the 20 ligands that bind to several targets (see fig 10 for illustration of the combination with Glide XP, Mango-III and DrugScore), there is a weak correlation between the DrugScore and Tversky similarity of interaction fingerprints, while there is a strong correlation between DrugScore and RMSD of ligand (R2 for linear least-squares regression equal 0.84).

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The software can be used for the characterization of the ligand’s and nucleic acid’s conformations. For this purpose, the trajectory fragments of biomolecules in the presence and in the absence of ligands are read, and two conformations are reconstructed. The software can either reconstruct a 3D model (using either the ligand’s 3D model or the nucleic acid’s 3D model from the trajectory), or it can provide a list of conformations (to be visualized with Jmol). The difference of a biomolecule’s conformations in a ligand-containing and a ligand-free trajectory indicates structural changes due to ligand’s presence. By reconstructing a biomolecule’s conformations, the software evaluates the ligand’s binding affinity to the receptor’s binding site in both the absence and presence of the ligand. This value represents the ligand’s binding affinity if the ligand was directly bound to the receptor’s binding site. It can be visualized together with the ligand in the active site or in the receptor’s binding site. Both the color scale and the values of the ligand’s binding affinity are calculated automatically based on the ligand’s 3D model or the nucleic acid’s model.] Evaluating poses predicted by molecular docking or pose prediction methods is often performed by analysis of docking scores (related to binding affinities) or by comparison of the ligand-protein complexes with the reference, including the quality of the shape of the ligand-protein complex or flexibility of the ligand conformation [85, 86]. However, this approach is not applicable when some compounds with desired properties do not interact with a specific part of the protein or the ligand is flexible in its conformation. Thus, we applied the fingerprint similarity to identify outliers in the predictions of Keplinger et al. [25]. We hypothesized that these outliers would be the compounds that do not follow the expected shape of the reference ligand-protein complex. To test this hypothesis, we selected the 11 groups of compounds that could not form interactions similar to that of the reference ligand (similarity below 0.2, and deviations larger than 3) as outliers and compared them to the active groups of Keplinger et al. [25]. We found that the 11 groups had to be represented by just one compound, which, in all cases, led to a shape similar to the reference ligand (Fig 7D), thus in agreement with the hypothesis. Therefore, the interactions formed by the reference conformation of the ligand may not have been properly predicted by the docking method. 5ec8ef588b

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