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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 (R^2 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 (R^2 for linear least-squares regression equal 0.84).

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Fingerprint clustering and visualization are complex tasks and require substantial programming effort. FINGERPRINT Jm180 does not permit complex analysis and visualizations of fingerprint structures. Such an analysis could be performed only at a large scale. We are in contact with the authors of the software mentioned above. We are interested in having access to the source code so that we can study its capabilities and seek improvements. We would be very grateful to be provided with it. Sequence features were extracted from protein sequences using custom software. Amino acid frequencies were calculated as the percentage of each residue in a given CAS type (see S17 Table). For variants not known to occur in the CAS types of interest, we substituted the residue at position 0 with a unique amino acid that does occur, as in the CASPER model developed by Naderi et al [48]. We also measured the frequency of amino acid pairs at every position in the protein. These measurements were saved in one-dimensional data vectors, each representing the average amino acid and amino acid pair frequency. When several CAS types are examined, it is possible that features derived from the CAS types with the fewest members (9 for *C. botulinum* proteomes in our dataset) are slightly favored because more CAS types may include some completely different amino acid pairs. To avoid potential over-fitting, we generated 21-dimensional feature vectors using all CAS types (*C. botulinum* CAS types with at least 10 members were excluded).

Data were normalized using the "normalize.quantiles" function from the ade4 package in R [54].

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