

Extensive reliability evaluation of docking-based target-fishing strategies

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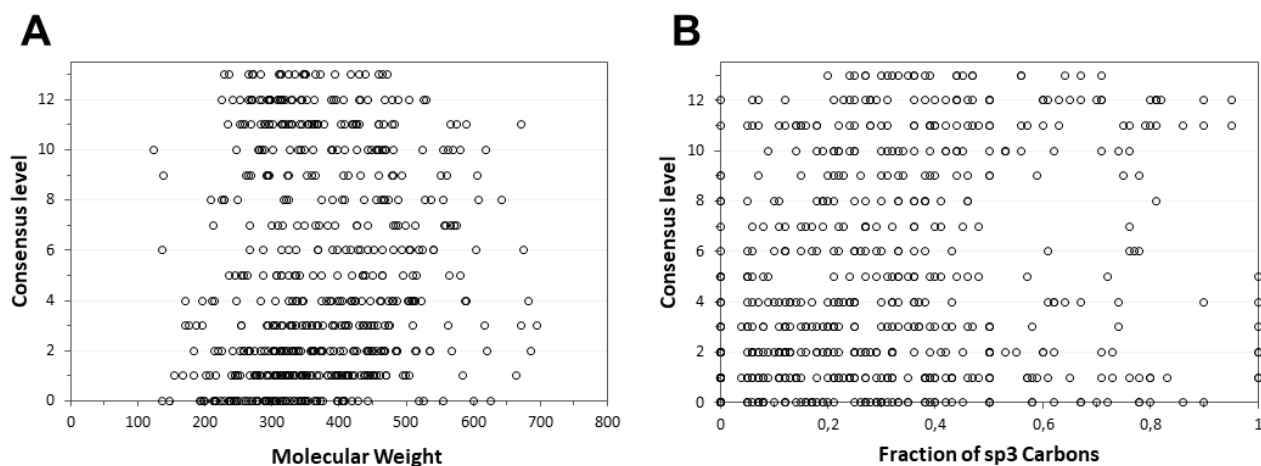


Figure S1. Analysis of consensus docking results in relation to ligand properties. Full data plots relative to (A) molecular weight and (B) fraction of sp3 carbons are reported, respectively.

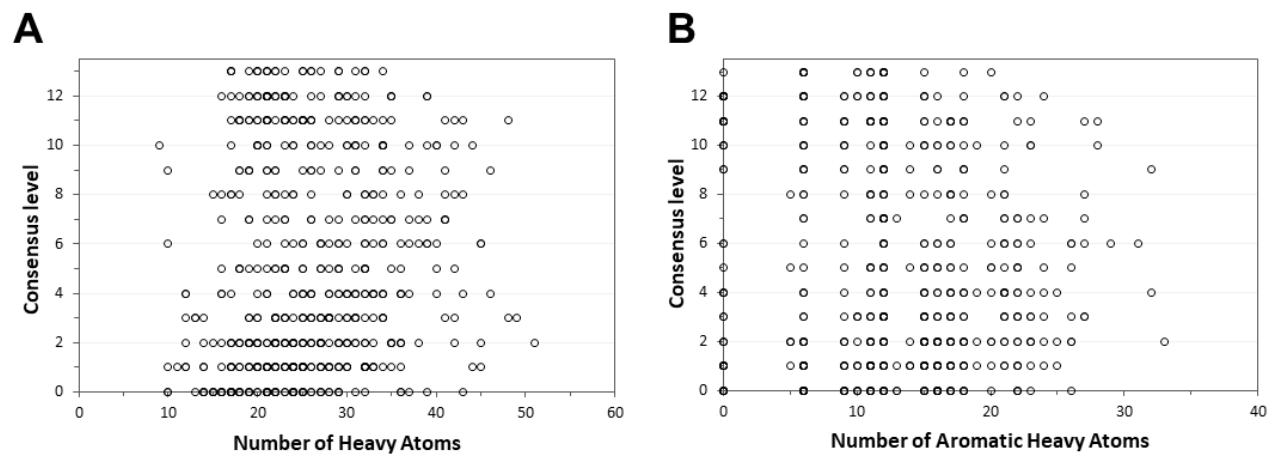


Figure S2. Analysis of consensus docking results in relation to ligand properties. Full data plots concerning (A) number of heavy atoms and (B) aromatic heavy atoms are reported, respectively.

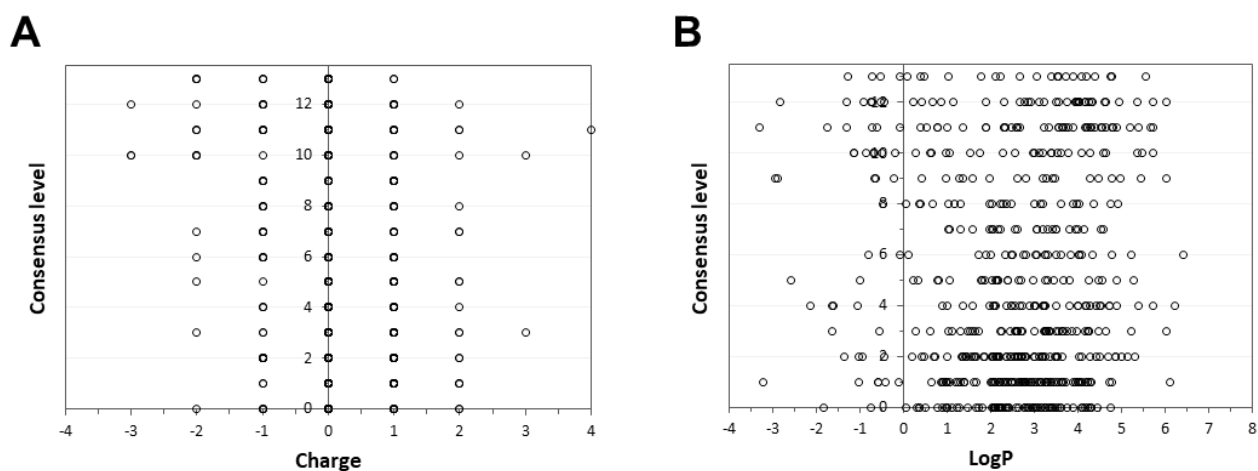


Figure S3. Analysis of consensus docking results in relation to ligand properties. Full data plots relative to (A) Charge and (B) LogP are reported, respectively.

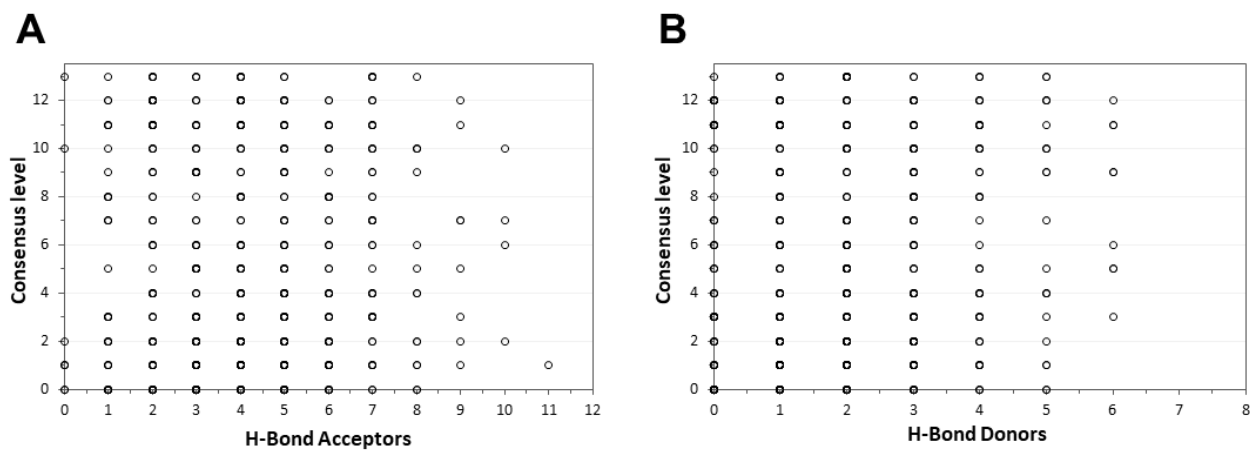


Figure S4. Analysis of consensus docking results in relation to ligand properties. Full data plots concerning (A) number of H-bond acceptors and (B) number of H-bond donors are reported, respectively.