ALiBERO: Evolving a team of complementary pocket conformations rather than a single leader

Manuel Rueda[1], Max Totrov[2] and Ruben Abagyan[1]

AUTHOR ADDRESS:

[1] Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, CA 92093, USA.

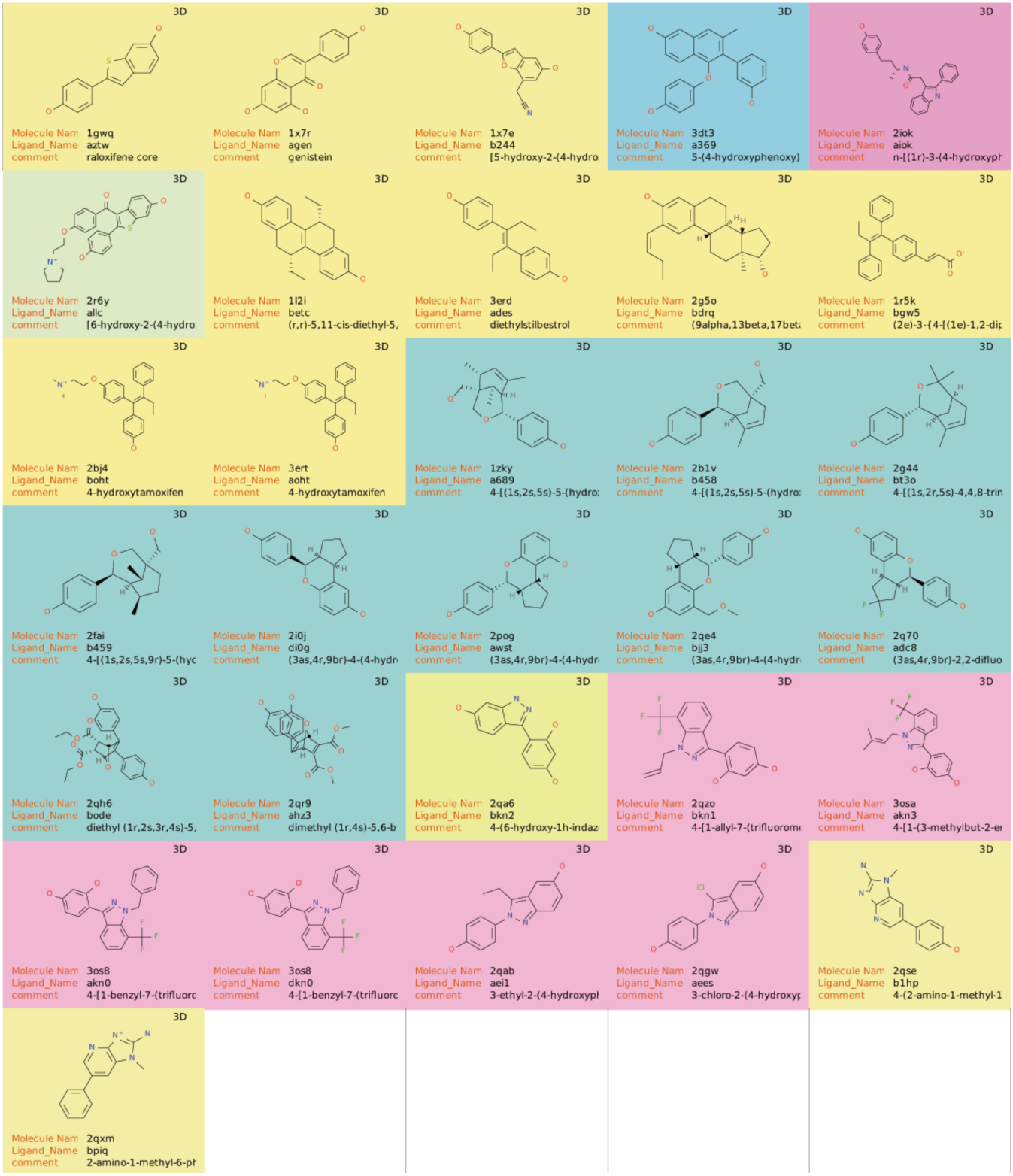
[2] Molsoft L.L.C., 11199 Sorrento Valley Road, S209, San Diego, CA 92121, USA.

AUTHOR EMAIL ADDRESS: rabagyan@ucsd.edu

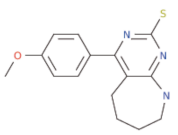
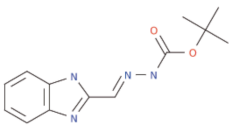
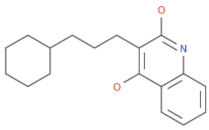
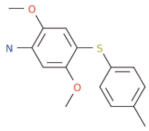
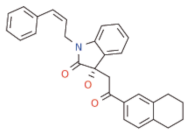
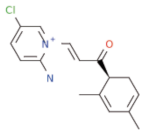
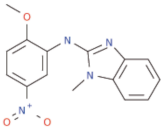
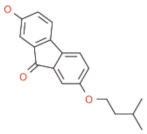
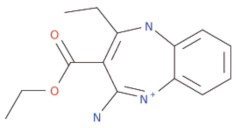
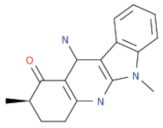
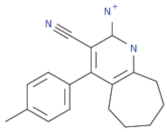
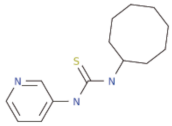
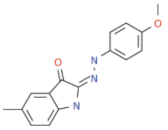
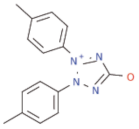
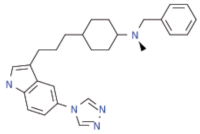
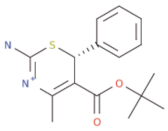
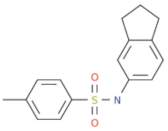
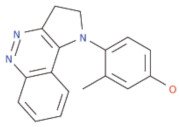
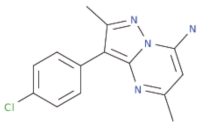
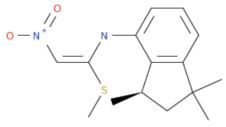
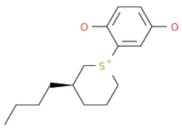
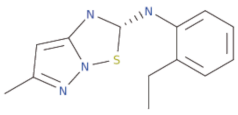
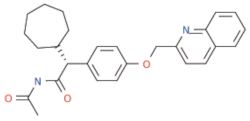
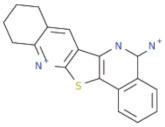
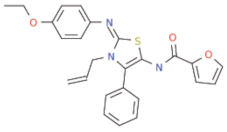
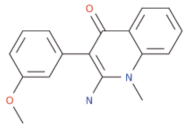
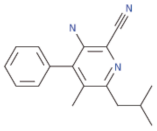
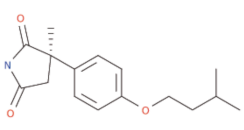
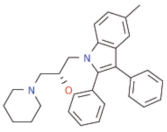
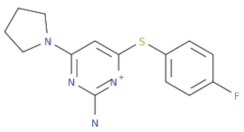
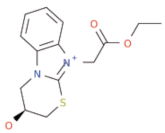
SUPPORTING INFORMATION AVAILABLE

Supporting Tables S1 and S2 including all compounds used in the training with ERα *($Tr_{1:1}$)* and Supporting Figure S3. This information is available free of charge via the Internet at http://pubs.acs.org.

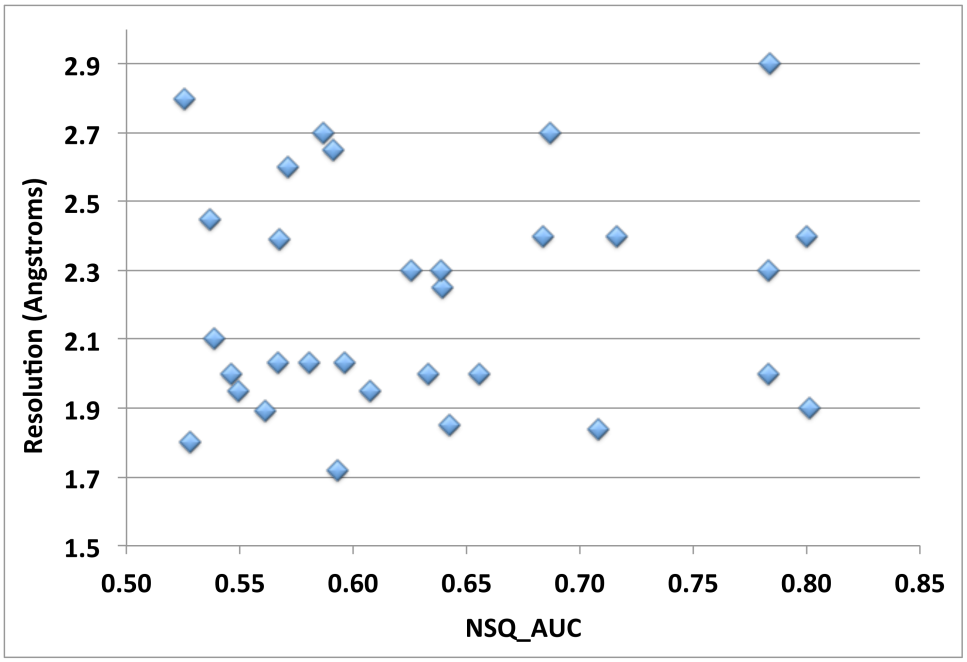
Supporting Table S1. List of the 31 active ligands (cognate ligands from the 31 PDB ID entries) used as training set ($Tr_{1:1}$) with the ERα protein.



Supporting Table S2. List of the 31 decoy compunds used as training set ($Tr_{1:1}$) with the ERα protein. The decoys were taken from Shoichet's directory of useful decoys (DUD) dataset.[1] The 31 ligands came from random selection among the 418 centroid clusters from all 4018 decoys in the entries "ER_agonist - Estrogen receptor agonist" and "ER_antagonist - Estrogen receptor antagonist").

3D  C15H17N3OS	3D  C13H16N4O2	3D  C18H23NO2	3D  C15H17NO2S	3D  C29H27NO3
3D  C16H18ClN2O	3D  C15H15N4O3	3D  C18H18O3	3D  C14H17N3O2	3D  C17H19N3O
3D  C18H21N3	3D  C14H21N3S	3D  C16H15N3O2	3D  C15H15N4O	3D  C27H34N5
3D  C16H20N2O2S	3D  C16H17NO2S	3D  C17H15N3O	3D  C14H13ClN4	3D  C15H21N2O2S
3D  C15H23O2S	3D  C13H16N4S	3D  C27H30N2O3	3D  C18H17N3S	3D  C25H23N3O3S
3D  C17H16N2O2	3D  C17H19N3	3D  C16H21NO3	3D  C29H33N2O	3D  C14H15FN4S
3D  C14H17N2O3S				

Supporting Figure S3. Plot showing the poor correlation between the x-ray resolution and screening performance for the 31 PDB ID entries present in the ESR1_HUMAN_300_551 pocketome entry.



REFERENCES

1. Huang, N.; Shoichet, B. K.; Irwin, J. J., Benchmarking sets for molecular docking. *J. Med. Chem.* **2006,** 49, (23), 6789-801.