Supporting Information

Scope of 3D shape-based approaches in predicting the macromolecular targets of structurally complex small molecules including natural products and macrocyclic ligands

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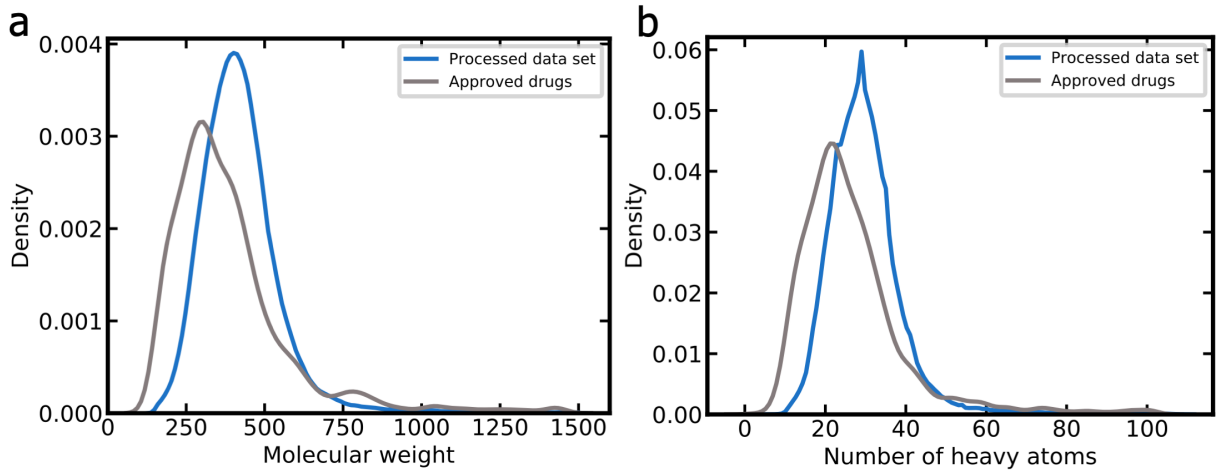

Figure S1. Density distribution of the (a) molecular weight and (b) the number of heavy atoms of all 481 194 compounds in the processed data set (blue; these are all valid compounds with at least one annotated bioactivity). The gray lines show the respective property distributions for the "Approved Drugs" subset of DrugBank[1] for reference.

REFERENCES

(1) Wishart, D. S.; Feunang, Y. D.; Guo, A. C.; Lo, E. J.; Marcu, A.; Grant, J. R.; Sajed, T.; Johnson, D.; Li, C.; Sayeeda, Z.; et al. DrugBank 5.0: A Major Update to the DrugBank Database for 2018. *Nucleic Acids Res.* **2018**, *46*, D1074–D1082.