

Title

Computer-aided pattern scoring – A multitarget dataset-driven workflow to predict ligands of orphan targets

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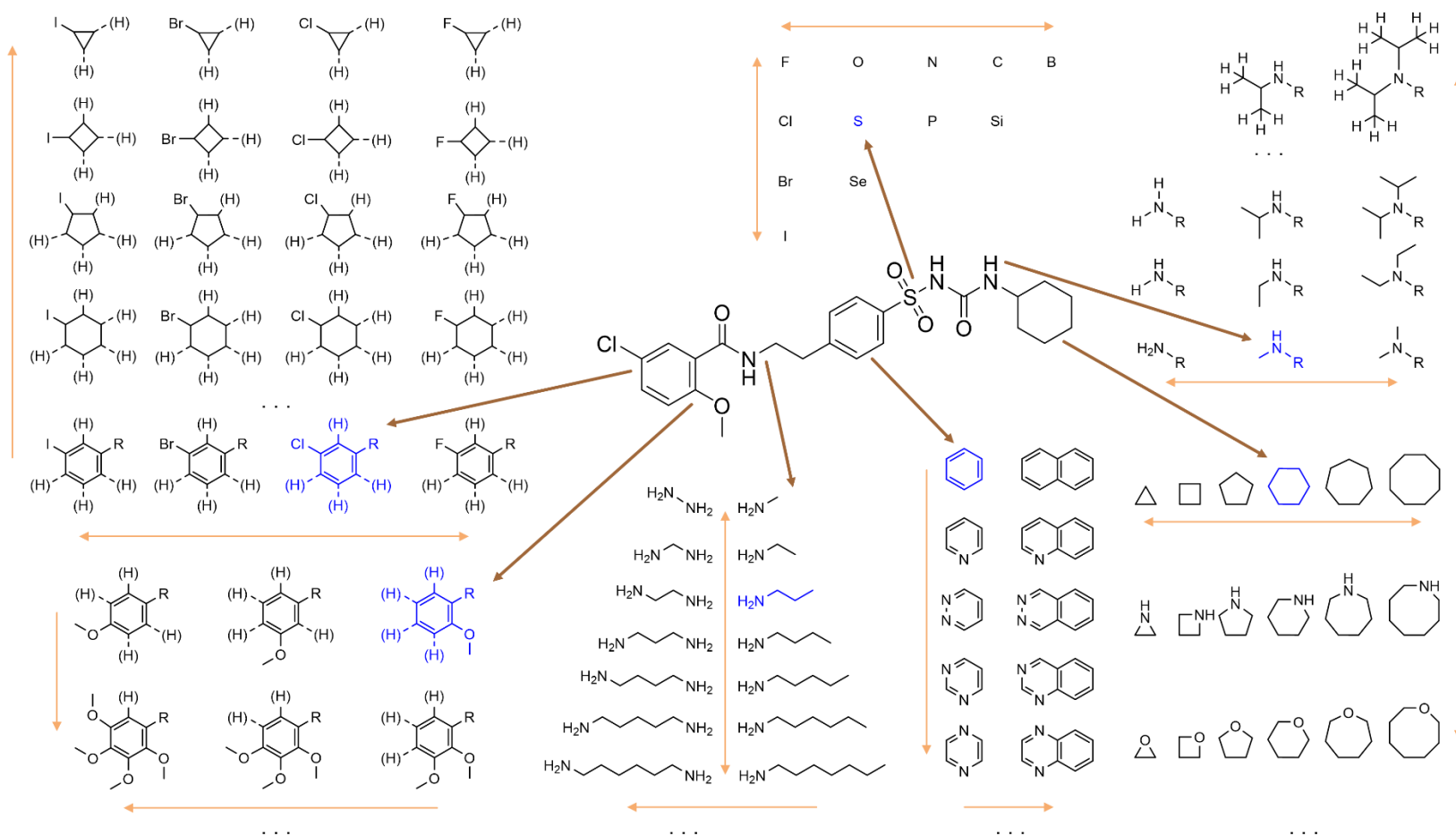
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Supplementary Information

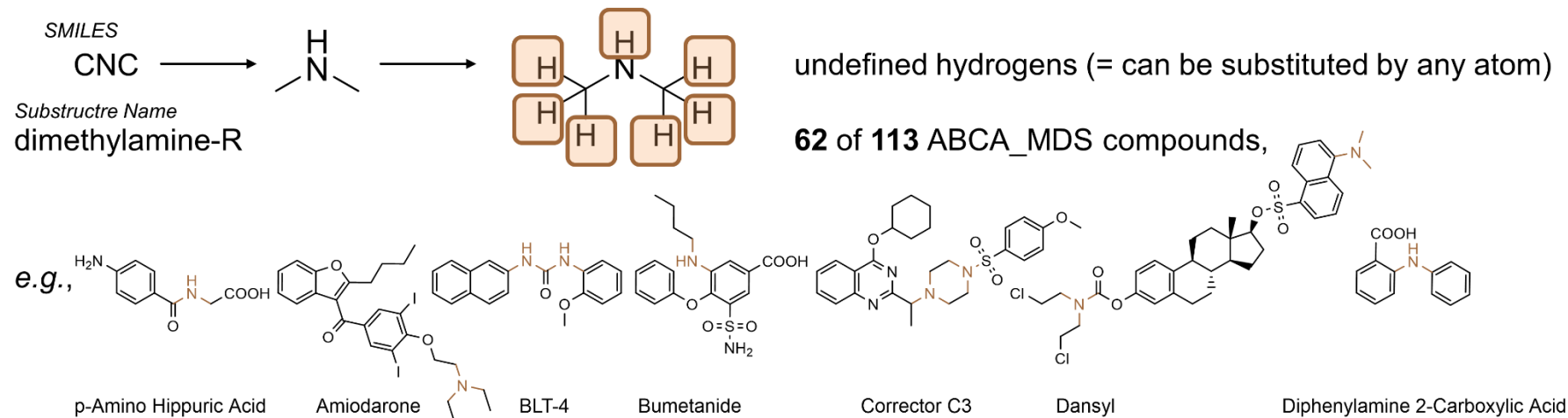
Supplementary Figure S1	P2
Supplementary Figure S2	P3
Supplementary Figure S3	P4



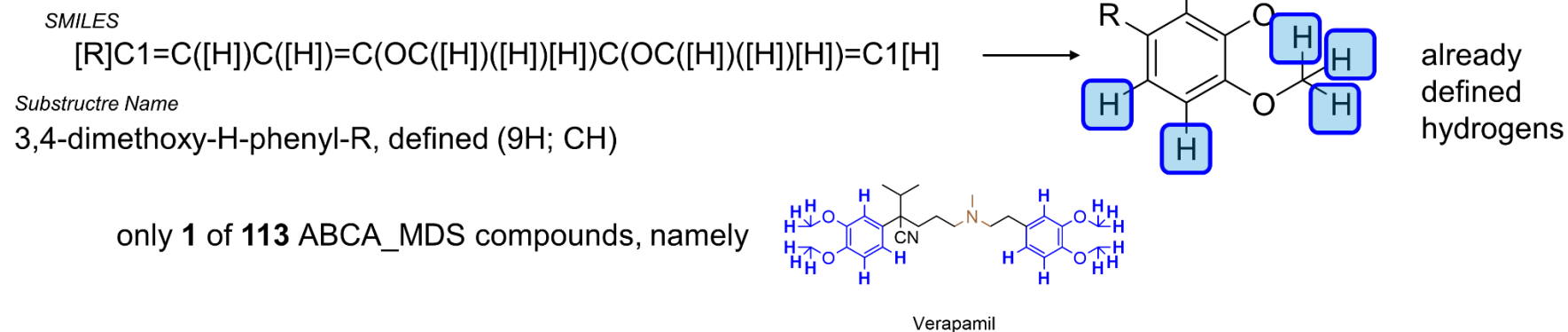
Supplementary Fig. 1 Visualization of the heavy atom distribution scheme as described earlier¹ using glibenclamide as example.

1. Namasivayam, V., Silbermann, K., Pahnke, J., Wiese, M. & Stefan, S.M. Scaffold fragmentation and substructure hopping reveal potential, robustness, and limits of computer-aided pattern analysis (C@PA). *Comput Struct Biotechnol J* **19**, 3269-3283, <https://doi.org/10.1016/j.csbj.2021.05.018> (2021)

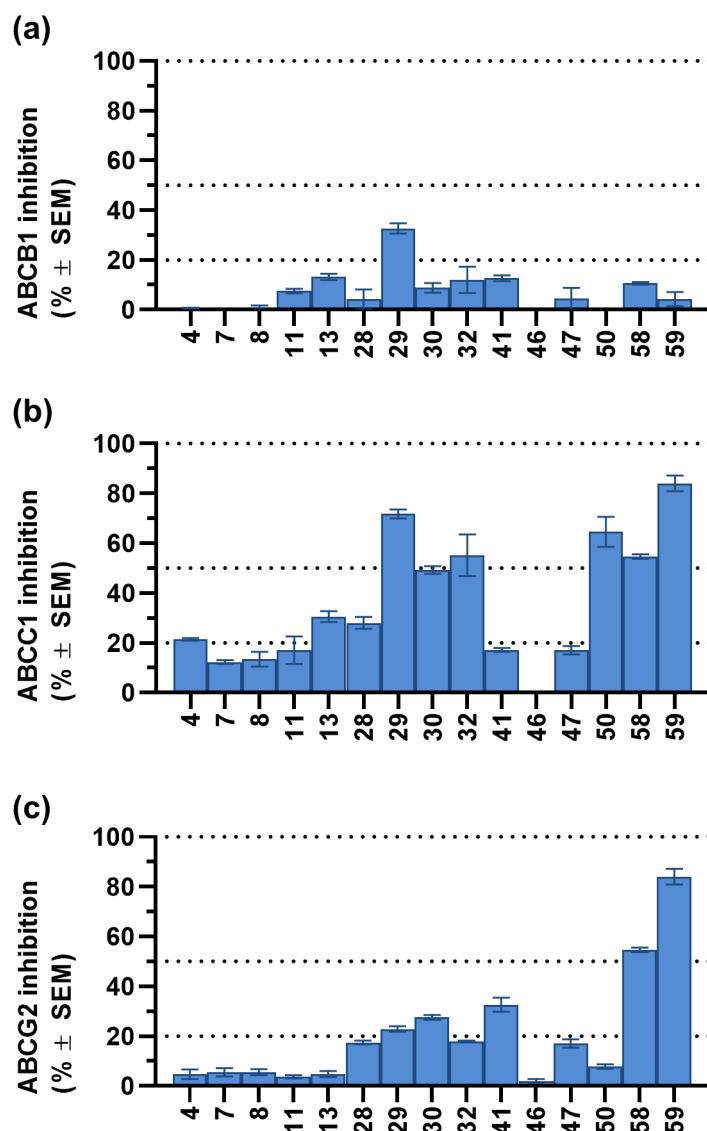
(a) Rather Unspecific Substructure:



(b) Rather Specific Substructure:



Supplementary Fig. 2 Visualization of rather unspecific (a) and rather specific (b) substructures.



Supplementary Fig. 3 Biological Assessment of hit compounds **4**, **7**, **8**, **11**, **13**, **28**, **29**, **30**, **32**, **41**, **46**, **47**, **50**, **58**, and **59** (10 μ M) against ABCB1 (a), ABCC1 (b), and ABCG2 (c) in calcein AM (a), daunorubicin (b), and pheophorbide A (c) assays using ABCB1-expressing A2780/ADR (a), ABCC1-expressing H69AR (b), and ABCG2-expressing MDCK II BCRP (c) cells as described earlier.²

- Möhle, L., *et al.* ABC Transporter C1 Prevents Dimethyl Fumarate from Targeting Alzheimer's Disease. *Biology (Basel)* **12** (7), 932, <https://doi.org/10.3390/biology12070932> (2023)