Supporting Information for

NP-Scout: Machine Learning Approach for the Quantification and Visualization of the Natural Product-Likeness of Small Molecules

Ya Chen 1, Conrad Stork 1, Steffen Hirte 1 and Johannes Kirchmair 1,2,3,*

1 Center for Bioinformatics (ZBH), Department of Informatics, Faculty of Mathematics, Informatics and Natural Sciences, Universität Hamburg, 20146 Hamburg, Germany; chen@zbh.uni-hamburg.de (Y.C.); stork@zbh.uni-hamburg.de (C.S.); steffen.hirte@studium.uni-hamburg.de (S.H.)
2 Department of Chemistry, University of Bergen, 5007 Bergen, Norway
3 Computational Biology Unit (CBU), Department of Informatics, University of Bergen, 5008 Bergen, Norway
* Correspondence: johannes.kirchmair@uib.no or kirchmair@zbh.uni-hamburg.de; Tel.: +47-5558-3464

Figure S1. Distribution of calculated NP-likeness scores for the DNP (after removal of any compounds present in the training set). Note that the y-axis is in logarithmic scale.