Exploration of Type II Binding Mode: a Privileged Approach for Kinase Inhibitor Focused Drug Discovery?

Supplemental information

Zheng Zhao¹, Hong Wu^{1,2}, Li Wang¹, Yi Liu³, Stefan Knapp^{4,5}, Qingsong Liu^{1,2}*, Nathanael S. Gray⁶*

¹High Magnetic Field Laboratory, Chinese Academy of Sciences, P.O. Box 1110, Hefei, Anhui 230031, P.R. China;

²University of Science and Technology of China, P. R. China, Anhui, Hefei, 230036

³Wellspring Biosciences LLC, 3210 Merryfield Row, San Diego, CA 92121;

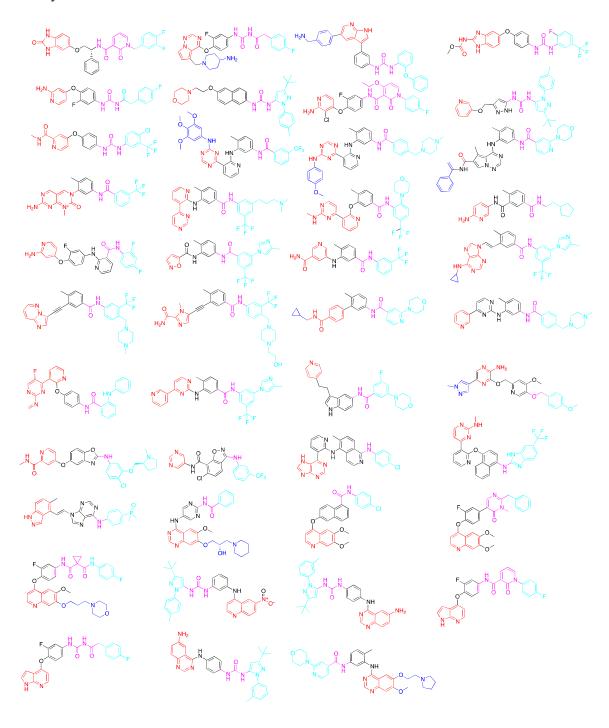
⁴Structural Genomics Consortium, University of Oxford, Old Road Campus Research Building, Roosevelt Drive, Oxford, OX3 7DQ, UK;

⁵Target Discovery Institute, University of Oxford, NDM Research Building, Roosevelt Drive, Oxford, OX37LD, UK

⁶Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, 250 Longwood Avenue, Boston, MA 02115, USA

*Correspondence: Qsliu97@hmfl.ac.cn (QL), nathanael_gray@dfci.harvard.edu (NSG)

Supplemental Fig. 1 type II kinase inhibitors extracted from DFG-out conformations of co-crystal structures.



Supplemental Fig. 2 Treespot representation of 12 selected type II kinase inhibitors

